September 2018

DERIVATION OF HUMAN HEALTH WATER QUALITY CRITERIA: REVIEW OF KEY SCIENTIFIC AND TECHNICAL ASSUMPTIONS AND APPROACHES SECOND EDITION

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Second Edition

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CONTENTS

TABLES

FIGURES

ATTACHMENTS

ACRONYMS AND ABBREVIATIONS

ADI	acceptable daily intake
BAF	bioaccumulation factor
BCF	bioconcentration factor
CSFII	Continuing Survey of Food Intake by Individuals
DOC	dissolved organic carbon
ELCR	excess lifetime cancer risk
FCM	foodchain multiplier
FCR	fish consumption rate
FDA	Food and Drug Administration
FDEP	Florida Department of Environmental Protection
g/day	grams per day
HHWQC	human health water quality criteria
HQ	hazard quotient
ICRP	International Commission on Radiological Protection
IDEQ	Idaho Department of Environmental Quality
L/day	liters per day
MCA	Monte Carlo Analysis
MCL	maximum contaminant level
MCLG	maximum contaminant level goal
mg/day	milligrams per day
NAS	National Academy of Sciences
NCI	National Cancer Institute
NHANES	National Health and Nutrition Examination Survey
NMFS	National Marine Fisheries Service
NOAA	National Oceanic and Atmospheric Administration
PAH	polycyclic aromatic hydrocarbon
PBT	persistent bioaccumulative toxins
PCB	polychlorinated biphenyl
POC	particulate organic carbon
PRA	probabilistic risk assessment
RfD	reference dose
RSC	relative source contribution
SDWA	Safe Drinking Water Act
ug/day	micrograms per day
USEPA	United States Environmental Protection Agency

FOREWORD

In June 2015 USEPA revised its recommendations for human health water quality criteria (HHWQC) for 94 substances. In doing so, USEPA changed most of the exposure-related assumptions used to derive the criteria, including the fish consumption rate, relative source contribution (RSC), bioaccumulation factors (BAFs), body weight, and drinking water consumption rate. Some of these changes do not reflect the best science, and nearly all States that have reviewed USEPA's revised criteria recommendations either have departed from them or are considering doing so in light of the better science provided by stakeholders and their urging that States use more representative assumptions for their States.

The Clean Water Act gives States the flexibility to reconsider the various assumptions used by USEPA for criteria development. The materials provided in this package are designed to encourage States to contemplate the criteria derivation process and thoughtfully consider designing criteria that provide a reasoned and transparent balance between theoretical risk, risk realities, and the implementation costs associated with potentially excessive conservatism in the criteria. Some of the areas where State-specific science choices may be preferred are highlighted below.

- Health Protection Targets. USEPA recommends a health protection target to protect the general population at between a one in one million ($1x10^{-6}$) and one in one hundred thousand ($1x10^{-5}$) increased lifetime cancer risk and that highly exposed sub-populations not exceed a one in ten thousand ($1x10^{-4}$) increased lifetime cancer risk. We encourage States to be specific about their health protection targets for at least the mean of the general population and higher-end exposure segment(s). Doing so recognizes the reality of the link between risk and exposure and allows more transparency and greater appreciation of actual risk associated with calculated HHWQC relative to other risks.
- Fish Consumption Rate. USEPA's 2015 HHWQC are based on a fish consumption rate of 22.0 grams per day (g/day). The prior recommendations were based on a fish consumption rate of 17.5 g/day. The difference in consumption rate is based primarily on two changes, neither of which suggests people are eating more fish in 2015 than they were in 2000. The first change results from an improved statistical method developed by the Centers for Disease Control that more accurately estimates lifetime fish consumption rates obtained from relatively short-term (several day) consumption surveys. The more accurate estimates are lower than USEPA's prior estimates. The second change involves adding marine fish and a portion of salmon consumption to the fish consumption rate. The basis for this addition is tenuous (at best), not transparent because USEPA will not release the data supporting its recommendation, and does not represent consumption of fish from waters of inland States that have no marine or estuarine waters.
- Relative Source Contribution. USEPA's recommended criteria for non-carcinogenic compounds include a relative source contribution (RSC) of between 20 and 80 percent. The value used for nearly all criteria before 2015 was 100 percent. The RSC acts to lower the HHWQC to account for exposures from other sources such that total exposure does not exceed toxicity thresholds. For most substances, the effect is to reduce (i.e., make more stringent) HHWQC by 5 times (if an RSC of 0.2 is used) compared to pre-2015 HHWQC. While ensuring that toxicity thresholds are not exceeded is important, USEPA's approach may be extreme and unwarranted in light of the numerous other conservative assumptions used to derive the criteria and especially when

substance-specific exposure data show little reasonable likelihood of other significant exposure pathways.

- Bioaccumulation Factor. USEPA's revised criteria are derived using substance-specific BAFs whereas the pre-2015 criteria were based on bioconcentration factors (BCFs). While a transition from BCFs to BAFs is consistent with accepted scientific consensus, the methodology USEPA used is not applicable to the waters of many States because it relies too heavily on models based on accumulation of polychlorinated biphenyls (PCBs) in the Great Lakes. PCBs are not representative of most of the substances for which criteria were revised, particularly in terms of metabolism and bioaccumulation potential, and USEPA has consistently stated that the Great Lakes are unique in their size, food web, temperature, historical pollutant loading and many other factors. States should evaluate whether USEPA's BAFs are appropriate for their waters.
- Drinking Water Ingestion. USEPA's revised criteria used an updated drinking water ingestion rate of 2.4 L/person/day. Thus, USEPA assumes that people drink this amount of water every day from untreated surface waters (or that treated drinking water contains substances at the criteria concentrations 100% of the time over a lifetime). States might consider whether this assumption is rational and appropriate for purposes of ambient water criteria.
- Other, Less Obvious, Exposure Assumptions. The revised criteria include several "implicit assumptions" (i.e., assumptions that affect the calculated criteria but are not parameterized in the criteria derivation equation). Examples include assuming that: all waters have a constant chemical concentration equal to the HHWQC; chemical concentrations are not reduced during cooking; people drink untreated surface water; and people consume fish and water with the maximum allowed contamination level continuously over their lifetime. These assumptions contribute to overstating exposure and risk. States should consider whether these assumptions are appropriate.
- Compounded Conservatism. Combining the conservative explicit and implicit assumptions described above leads to a phenomenon referred to as "compounded conservatism" wherein the level of protection afforded by HHWQC is far greater than stated health protection targets. This phenomenon should be recognized and thoughtfully considered in light of the implementation costs and potential for misallocation of public and private resources associated with excessive conservatism in the criteria.
- Probabilistic Risk Assessment. The 2015 National HHWQC use a decades-old risk assessment approach for which alternatives both exist and are preferred by the modern risk assessment community. The preferred approach, now adopted by at least one State in deriving HHWQC, is probabilistic risk assessment (PRA). Among the advantages of PRA is that it uses more of the available data and that it creates a rational and transparent link between the criteria and specific health protection targets. Thus, PRA allows States to confirm that they have achieved their stated health protection goals.

The level of effort required to address many of the most critical of the above issues is not large. For example:

- Long-term fish consumption rates for different regions of the country are available (see, for example, *Estimated Fish Consumption Rates for the U.S. Population and Selected Subpopulations (NHANES 2003-2010), Final Report*. EPA-820-R-14-002. April 2014)

- Florida has reviewed exposure data for 26 compounds and developed RSCs and other researchers have published RSCs (see, for example, Appendix D of the *Technical Support Document: Derivation of Human Health-Based Criteria and Risk Impact Statement.* Florida Department of Environmental Protection, June 2016);
- BAFs are a critical input only for bioaccumulative compounds and information is available for several inputs to refine USEPA's procedure to make it more applicable to State waters (see, for example, Attachment F: *Review of PAH Bioaccumulation and Bioconcentration Factors used by USEPA in Derivation of 2015 Human Health Water Quality Criteria*; and Attachment L: *Refinement of Foodchain Multipliers and Bioaccumulation Factors used by USEPA to Derive 2015 Water Quality Criteria*
- Software tools are available that enable the use of PRA to derive HHWQC (see, for example, Attachment J to this report: *Probabilistic Approach to Deriving Ambient Water Quality Criteria White Paper*.

EXECUTIVE SUMMARY

USEPA's 2015 National Human Health Water Quality Criteria (HHWQC) included revisions to many of the inputs used to derive the pre-2015 National HHWQC. Some of the revisions were based on new science and data, others were based on science policy decisions, and others were a mix of the two. This report presents background information on many of those inputs with a focus on new data and science. The goal of the background information is to provide State regulators a broader perspective of the data and science surrounding these inputs and, in the process, identify areas where the assumptions used by USEPA to develop the 2015 National HHWQC may not reflect the best science and/or may not be applicable to the waters of specific States. States may wish to consider this information when establishing State-specific HHWQC that meet their human health protection targets and are based on the best science available. The remainder of the Executive Summary provides an overview of the information discussed in each of the sections of this report.

Health Protection Targets

USEPA's 2015 National HHWQC are based on a health protection target of a one in one million ($1x10^{-6}$) increased lifetime cancer risk, over and above background (an increase from about 40.0000% to 40.0001%). USEPA's guidance recommends HHWQC protect the general population at between a $1x10^{-6}$ and one in one hundred-thousand ($1x10^{-5}$) increased lifetime cancer risk. It further recommends that highly exposed populations not exceed a one-in-ten-thousand ($1x10^{-4}$) increased lifetime cancer risk. Given that these health protection targets are very small compared to the daily risk of accidental (involuntary) death faced by everyone in the United States and will result in immeasurable changes in overall cancer incidence, they confer a high level of protection. Yet a choice of $1x10^{-6}$ versus $1x10^{-5}$ will result in a 10-fold difference in HHWQC. This represents a larger change in HHWQC than is likely to be associated with any other individual assumption that affects HHWQC.

Selection of the health protection target is primarily a risk management decision and not exclusively a science decision. Each State may have its own health protection targets consistent with its own risk management and public health protection policies. This report provides background on the use of one in one million and other allowable risk levels in other regulatory programs. Accepting that the Clean Water Act may have unique risk management considerations compared to other statutes and regulations, it remains informative to compare allowable risk levels used by a range of statutes and regulations. The report also provides information on the predicted increase in cancer incidence in the exposed population associated with different allowable risk levels and compares that increase to background cancer incidence associated with other causes. Such comparisons provide perspective regarding the overall improvement in public health achieved by HHWQC using different allowable risk levels. States may wish to carefully consider the cumulative effect of all the assumptions used to derive State-specific HHWQC when selecting health protection targets.

Fish Consumption Rate

USEPA's 2015 National HHWQC assume a fish consumption rate (FCR) of 22.0 grams per day (g/day). The pre-2015 HHWQC were based on a fish consumption rate (FCR) of 17.5 g/day. The difference in

consumption rate appears to be based primarily on two changes. Interestingly, neither of those changes suggests that people are eating more fish in 2015 than they were during the prior 15 years. The first change involves the methodology used to estimate long-term (lifetime) consumption rates from relatively short-term (several day) consumption surveys. Pre-2015 HHWQC used FCRs reported by short-term surveys. In the past decade researchers realized short-term fish consumption rate information is not representative of long-term consumption rates. Short-term surveys overpredicted long-term consumption of the upper percentiles of the population and underpredicted long-term consumption of lower percentiles. Scientists at the National Cancer Institute (NCI) developed a methodology to correct this bias and predict long-term consumption from short-term survey information. USEPA applied a similar methodology to develop the FCRs used to establish the 2015 National HHWQC[1]. The effect of applying the method is to improve the accuracy of the FCR for the upper percentiles.

The second change was to include some marine fish and a portion of salmon consumption in the overall fish consumption rate. Prior to 2015, marine fish and salmon were excluded from the consumption rate used to establish National HHWQC because such fish were assumed to accumulate little or none of their body burden from estuarine and freshwaters (i.e., the waters in which chemicals concentrations can be affected by HHWQC). When developing the FCR for the 2015 National HHWQC, USEPA included some marine fish based on the assumption that some marine species spend a portion of their life history in near-shore waters and during that time accumulate chemicals from such waters. For similar reasons a portion of salmon consumption was also included. However, USEPA has provided long-term consumption rates for various groups of species and not individual species, which makes it impossible to determine how much of the increase in fish consumption rate (from 17.5 g/day to 22 g/day) is related to application of the NCI methodology and how much is due to inclusion of marine species. Given that the NCI methodology reduces the high bias in the upper percentiles (e.g., 90th, 95th) of fish consumption rates from short-term surveys, it is likely that application of the NCI methodology alone would have led to a decrease in the estimated 90th percentile fish consumption rate to a rate of less than 17.5 g/day. Inclusion of salmon and other marine species may, therefore, explain why the 90th percentile FCR used by USEPA to derive the 2015 National HHWQC increased from 17.5 g/day to 22 g/day. USEPA's lack of transparency regarding species-specific FCRs will create a challenge for States to use the USEPA FCR data and develop FCRs representative of the fish species consumed from a State's waters. However, it bears pointing out that USEPA (2014a) does provide information on the long-term FCR of just freshwater finfish and shellfish (summarized for different regions of the US in Table 2); these rates may be applicable to States with no estuarine or near-shore waters.

Relative Source Contribution

For most chemicals, when evaluating the non-carcinogenic endpoint, USEPA's 2015 National HHWQC use a default relative source contribution (RSC) of 0.2. For most of the same chemicals, USEPA used an RSC of 1.0 when setting HHWQC prior to 2015. The effect of the change is to decrease the HHWQC for

[1] To distinguish between fish consumption rates reported by fish consumption surveys from long-term fish consumption rates derived using the NCI (or similar) method, USEPA has developed the term Usual Fish Consumption Rate (UFCR). UFCR is used to represent long-term fish consumption rates derived using the NCI method. Thus, fish consumption rates used in HHWQC prior to 2015 are referred to by USEPA as FCRs and those used in the 2015 HHWQC are referred to as UFCRs. For simplicity, this report uses FCR, even when referring to long-term fish consumption rates derived using the NCI method.

such chemicals by five-fold. The concept of the RSC has a long history starting in the 1970s with the National Academy of Sciences considering how to set drinking water standards and as early as 1980 with the USEPA setting HHWQC. The concept of an RSC has been applied to drinking water standards for several decades. However, prior to 2015, USEPA used an RSC of 1 for most chemicals when setting HHWQC, despite having developed in 2000 an extensive discussion and framework for application of RSCs when deriving HHWQC. That framework describes two different methods (i.e., the subtraction and the percentage methods) that can be used to derive RSCs as well as conditions under which one or the other method is preferred. RSCs resulting from the two methods can vary a great deal and the basis for the conditions set forth by USEPA is not always clear. That means States may need to consider carefully whether available data support the RSCs used by USEPA to derive the 2015 National HHWQC and whether USEPA's RSCs should be used when deriving State-specific HHWQC.

Bioaccumulation Factors

To estimate the accumulation of chemicals in fish and shellfish USEPA's 2015 National HHWQC use bioaccumulation factors (BAFs) rather than bioconcentration factors (BCFs). Theoretically, BCFs account for uptake from just water, whereas BAFs account for uptake from all pathways (e.g., water, diet, and sediment). The switch from BCFs to BAFs is consistent with the consensus in the scientific community that accumulation of most chemicals can be better predicted by accounting for uptake from all exposure pathways rather than just from water. However, the complicating factor with BAFs is that they depend upon many water body-specific characteristics including dissolved and particulate carbon, temperature, sediment profiles and food web structure. All of these conditions can vary greatly between waters and, thus, so too can BAFs. To estimate National BAFs for the 2015 HHWQC, USEPA used a methodology that relies heavily on a model of PCB accumulation in the Great Lakes. USEPA stated repeatedly when discussing the need for the Great Lakes Initiative in the 1990's, that the Great Lakes represent a set of waters and food web so unique that they need their own unique criteria. Compared to other state waters, differences in the species present in the food web, ambient water temperatures, and the ratio of regulated substances found in the sediment versus the water column may all substantially affect the development of regionally specific BAFs. As well, the assumptions made regarding metabolism in the Great Lakes PCB model lead to the overestimation of bioaccumulation for most other substances. Thus, a bioaccumulation model based on PCBs in the Great Lakes is not applicable to all waters in the United States. To address this deficiency, and ease the burden in re-running USEPA's bioaccumulation model, information is provided in this report that can be easily applied by a State or interested party to generate state-specific BAFs that better represent chemical behavior and local conditions.

Assumed Concentration of Receiving Waters

USEPA's derivation of HHWQC assumes that all surface water has a chemical concentration equal to the HHWQC at all times. The assumption is unlikely to be true for freshwater and is even less likely to be true for estuarine and near-shore waters for several reasons. First, typical regulatory permit requirements result in chemical concentrations at the compliance point that are lower than the HHWQC. Because of additional dilution beyond the compliance point, concentrations will be even lower in the receiving water beyond the compliance point. Second, once flowing waters reach an estuary or near shore water, additional dilution will occur based just on the volume of saltwater compared to freshwater inputs. Third,

beyond volume, additional mixing occurs because of tides, wind driven currents, and currents associated with larger oceanic circulation. Thus, the assumption of a constant surface water concentration equal to the HHWQC adds conservatism that is not explicitly accounted for by the parameters listed in the HHWQC derivation equations. When setting State-specific HHWQC, States may wish to consider whether and how to account for the overestimation of exposure and risk associated with this implicit assumption.

Other Assumptions and Parameters

USEPA updated several other assumptions when establishing the 2015 National HHWQC. Those include increasing the drinking water ingestion rate from 2.0 liters per day (L/day) used by the pre-2015 HHWQC to 2.4 L/day and increasing body weight from 70 kilograms (kg) to 80 kg. Those changes are consistent with updates USEPA has made in other regulatory programs for those two parameters. However, it should be noted that use of this value to derive HHWQC embodies the assumption that all people effectively use untreated surface water as a drinking water supply which, of course, is far from realistic.

With the exception of the assumed concentration of a chemical in surface water, all of the assumptions discussed in this paper are explicitly shown in the equations used to calculate HHWQC. However, several assumptions are implicit in the calculation of HHWQC, in addition to the assumption that all waters have a concentration equal to the HHWQC all the time. Other implicit assumptions include that the chemical concentration in fish does not change during cooking and that all water that people drink is obtained from untreated surface water, among others. Both of those assumptions add to the conservatism of HHWQC. Recognizing the existence of implicit assumptions that add to the conservatism of HHWQC has the potential to affect how some States manage the overall conservatism inherent in HHWQC.

Compounded Conservatism and PRA

Collectively, using multiple conservative assumptions results in HHWQC that may be far more protective than necessary to meet the risk management goal used to derive the HHWQC. This phenomenon of greater conservatism embodied by the whole rather than the conservatism of each individual part is referred to as "compounded conservatism." In the HHWQC derivation process, compounded conservatism plays a role both in the determination of individual factors of the derivation equations (i.e., in the toxicity factors and explicit and implicit exposure elements) and in the equations' use of multiple factors, most based on upper bound limits and/or conservative assumptions.

Estimating the degree of conservatism inherent to HHWQC is impossible using the standard deterministic risk assessment approach. In that approach, a single value is used for each parameter and then the standard equation is solved for the surface water concentration that results from those inputs. The resulting surface water concentration is the HHWQC. From that calculation, it is impossible to know to which percentile of the population the estimated risk applies (e.g., the 90th, 99th, 99.99th, etc.) and, therefore, whether and by how much the resulting HHWQC is over- or under-protective relative to the stated health protection targets.

Application of probabilistic risk assessment methods can help quantify the level of protection afforded different segments of the exposed population and, consistent with USEPA's goals regarding transparency, makes the HHWQC process far more transparent than the standard deterministic approach. In the past, the information and computational requirements associated with probabilistic

methods would have posed a challenge to most States. However, as discussed in this report, data on the input distributions of most of the key inputs are available as are computational tools to facilitate derivation of HHWQC using probabilistic methods.

Summary

In summary, a priori, one cannot predict whether consideration of the information presented in this report, and other information States may have available to them to establish scientifically defensible inputs, will result in State-specific HHWQC that are higher or lower than USEPA's 2015 National HHWQC. Given the large number of inputs upon which HHWQC depend, the diversity of waters, food webs, and characteristics of State-populations across the United States, and the large number of chemicals involved, it is likely that some State-specific HHWQC will be higher than USEPA's 2015 National HHWQC and others will be lower. The goal of this report is to provide States with information that allows them to establish State-specific HHWQC that meet each States' human health protection targets and are based on the best science available.

1 INTRODUCTION

This report is intended assist States in their review and consideration of USEPA's recommended water quality criteria for protection of human health (USEPA 2015a). The focus of this report is on technical and not policy/legal issues, though some of the information presented could be used by States to inform their policy/legal choices, particularly with respect to selecting human health risk protection targets (i.e., allowable risk levels) and addressing matters related to compounded conservatism in USEPA's recommended criteria.

As described in USEPA (2015a), HHWQC are derived using one of four standard equations, depending upon whether the chemical is assumed to cause non-cancer or cancer effects, and depending upon whether the HHWQC are being set to protect against adverse effects associated with consumption of water and organisms or to protect against adverse effects associated with consumption of organisms only. The equations and inputs are shown below.

Non-cancer effects, water and organisms:

$$HHWQC = THQ \times RfD \times RSC \times \left(\frac{BW}{DI + \sum_{i=2}^{4}(FCR_i \times BAF_i)} \right)$$

Non-cancer effects, organisms only:

$$HHWQC = THQ \times RfD \times RSC \times \left(\frac{BW}{\sum_{i=2}^{4}(FCR_i \times BAF_i)} \right)$$

Cancer effects, water and organisms:

$$HHWQC = TELCR \times \frac{1}{CSF} \times \left(\frac{BW}{DI + \sum_{i=2}^{4}(FCR_i \times BAF_i)} \right)$$

Cancer effects, organisms only:

$$HHWQC = TELCR \times \frac{1}{CSF} \times \left(\frac{BW}{\sum_{i=2}^{4}(FCR_i \times BAF_i)} \right)$$

Where:

HHWQC = human health water quality criterion (mg/L);
THQ = target hazard quotient (unitless);
TELCR = target excess lifetime cancer risk (unitless);
DI = drinking water intake (L/day);
FCR_i = trophic level-specific fish consumption rate (kg/day);
BAF_i = trophic level-specific bioaccumulation factor (L/kg tissue);
BW = bodyweight (kg);
RSC = relative source contribution (unitless);
RfD = reference dose (mg/kg-day); and
CSF = cancer slope factor $(mg/kg\text{-}day)^{-1}$.

Each section of this report discusses one or more of the inputs shown in the above equations. Section 2 discusses the fish consumption rate, Section 3 the relative source contribution, Section 4 the

bioaccumulation factor (BAF), Section 6 the drinking water intake and bodyweight, and Section 9 the human health protection targets. This report does not discuss the basis and background of toxicity parameters (i.e., the reference dose and cancer slope factor) given that those are derived by USEPA outside of the Clean Water Act and are generally accepted and used by all USEPA programs. That does not preclude States from deriving and using their own toxicity factors (e.g., CalEPA 2009, 2015), though for most States the resources required to do so may be prohibitively large. The report also discusses some assumptions that are not explicitly included in the above equations but are implicit in the derivation of HHWQC. Those include assumptions about the concentration of chemicals in receiving water (discussed in Section 5), the absence of a change in chemical concentration during cooking and that drinking water is untreated (both of the latter assumptions are discussed in Section 6).

In addition to discussion of the input assumptions, Section 7 describes how the typical approach to derivation of HHWQC (used by USEPA when deriving the 2015 National HHWQC as well as by virtually all States, with the exception of Florida, when setting their current HHWQC) leads to compounded conservatism, which results in HHWQC that are more protective than indicated by the human health protection target used to set the HHWQC. This report then discusses the benefits of using a probabilistic approach (Section 8) when deriving HHWQC to address and quantify the effects of compounded conservatism and improve transparency. Section 9 summarizes some information on background risk to provide perspective on the selection of health protection targets. Finally, this report includes a series of attachments. The attachments provide more detailed discussion of many of the input parameters discussed in the main body of the report.

2 FISH CONSUMPTION RATE

Derivation of HHWQC depends upon many input assumptions. Likely none have received more attention than selection of the fish consumption rate (FCR). This section (and associated attachments) review recent developments in our understanding of FCRs. The section identifies key issues that States may wish to consider when deciding whether to base a State-specific HHWQC on the same FCR that USEPA used in the 2015 National HHWQC (USEPA 2015a), or whether to use State-specific or other data to develop a FCR representative of the fish consumption habits of State residents.

2.1 Fish Consumption Rate

HHWQC are developed to protect people from lifetime exposure to chemicals in surface water. Over the last decade or two, scientists have come to realize that FCRs observed during short-term dietary surveys are not representative of a person's lifetime FCR. Variations over time in the consumption habits of individuals can be substantial, particularly for episodically consumed foods such as fish. Because HHWQC are derived based on a lifetime of exposure, developing long-term average FCRs from short-term dietary survey data is critical[2]. Researchers at the National Cancer Institute (NCI) developed a statistical methodology to estimate FCRs from repeated short-term dietary surveys. The NCI method

[2] As noted above, USEPA refers to long-term fish consumption rates (i.e., those that may be representative of a lifetime of consumption) as usual fish consumption rates (UFCRs). However, for consistency with the parameters used in the HHWQC derivation equations, this report will refer to such long-term fish consumption rates simply as fish consumption rates (FCRs).

provides distinct advantages over previously proposed methods by accounting for days without consumption, distinguishing within-person variability from between-person variation, allowing for the correlation between the probability of consuming a food and the consumption per day amount, and relating covariate information to usual intake (Tooze et al. 2006). USEPA in its 2015 update and Idaho Department of Environmental Quality (IDEQ) have recently used the NCI method to develop estimates of fish consumption (USEPA 2014a, NWRG 2016); USEPA, IDEQ, and Florida Department of Environmental Protection (FDEP) have recently employed FCRs (i.e., consumption rates assumed to represent long-term consumption behavior rather than consumption rates from short-term surveys that may result in biased estimates of consumption) to derive HHWQC (USEPA 2015a, IDEQ 2016, FDEP 2016).

USEPA has developed national FCRs as well as FCRs for 14 regions of the country (Table 1). The FCRs for various regions of the country differ from the 22.0 grams per day (g/day) FCR for freshwater and estuarine fish and shellfish used by USEPA to derive the 2015 National HHWQC (USEPA 2015a). The FCRs for coastal regions tend to be greater than the FCR of 22.0 g/day used by USEPA to represent the whole country; the FCRs for inland regions tend to be lower – for some regions, substantially lower (13.5 g/day for the Inland Midwest at the 90th percentile versus 22.0 g/day for the nation as a whole (Table 1). These data suggest that even if States do not have recent fish consumption rate survey data that could be used to develop State-specific FCRs (as did Idaho), States can use region-specific FCRs rather than the national FCR of 22 g/day to better represent fish consumption within a State. States that have areas with varying fish consumption habits (e.g., coastal counties and inland counties) could consider developing a State-specific FCR based on weighting FCRs according the size of population in counties with applicable regional FCRs. Florida employed such an approach when deriving State-specific HHWQC (FDEP 2016).

Table 1. National and Regional Fish Consumption Rate Estimates for Freshwater and Estuarine Finfish and Shellfish

Population	Mean (grams/day)	Percentile (grams/day)						
		25th	50th	75th	90th	95th	97th	99th
National								
National	9.2	1.8	5.0	11.4	22.0	31.8	40.2	61.1
Region[1]								
Northeast	9.7	2.1	5.8	12.6	23.1	32.3	39.9	58.5
Midwest	6.0	1.2	3.2	7.4	14.3	20.8	26.3	41.1
South	11.0	2.4	6.4	14.0	26.3	37.5	46.7	69.0
West	9.5	1.9	5.1	11.4	22.4	32.7	42.0	66.9
Coastal Status[2]								
Noncoastal	7.9	1.5	4.2	9.8	19.0	27.4	34.6	52.8
Coastal	11.5	2.6	6.6	14.4	27.1	38.6	48.4	72.7
Coastal/Inland Region[3]								
Pacific	11.6	2.4	6.3	14.0	27.3	39.7	51.2	81.2
Atlantic	13.3	3.5	8.3	17.0	30.8	42.8	52.3	75.8
Gulf of Mexico	12.2	2.8	7.3	15.7	28.6	40.1	50.3	73.8
Great Lakes	6.9	1.5	4.0	8.7	16.5	23.6	29.4	44.5
Inland Northeast	8.7	1.7	5.0	11.3	21.0	29.5	36.5	54.4
Inland Midwest	5.7	1.1	3.0	6.9	13.5	19.8	25.1	39.5
Inland South	9.5	1.9	5.3	12.0	22.8	32.7	40.9	61.0
Inland West	7.7	1.7	4.3	9.4	18.2	26.3	33.3	51.6

Notes:

Fish consumption rate estimates are total freshwater and estuarine finfish and shellfish usual fish consumption rate estimates, raw weight, edible portion, for adults.

1. U.S. Census Regions
   Midwest = OH, MI, IN, WI, IL, MO, IA, MN, SD, ND, NE, and KS
   Northeast = PA, NY, NJ, CT, RI, MA, NH, VT, and ME
   South = DE, MD, DC, VA, WV, KY, TN, NC, SC, GA, AL, MS, FL, LA, AR, OK, and TX
   West = NM, CO, WY, MT, ID, UT, AZ, NV, CA, OR, WA, AK, and HI
2. All counties that bordered the Pacific or Atlantic Oceans, the Gulf of Mexico or any of the Great Lakes were defined as coastal. Additionally, counties that bordered estuaries and bays were defined as coastal as were counties whose centroid was within approximately 25 miles of any coast even if not directly bordering a coast.
3. Coastal and Inland Regions
   Pacific Coast = coastal counties in CA, OR, WA, AK, and HI
   Atlantic Coast = coastal counties in CT, DE, DC, FL (bordering Atlantic Ocean), GA, ME, MD, MA, NH, NJ, NY, NC, PA, RI, SC, and VA
   Gulf of Mexico Coast = coastal counties in AL, FL (bordering Gulf of Mexico), LA, MS, and TX
   Great Lakes Coast = counties bordering the Great Lakes in MI, WI, OH, NY, MN, IN, IL, and PA
   Inland West = remaining counties in CA, OR, WA, AK, and HI and all of NM, CO, WY, MT, ID, UT, AZ, and NV
   Inland South = remaining non-coastal counties in DE, MD, DC, VA, NC, SC, GA, AL, MS, FL, LA, and TX and all of WV, KY, TN, AR, and OK
   Inland Northeast = remaining counties in PA, NY, NJ, CT, RI, MA, NH, and ME and all of VT
   Inland Midwest = remaining counties in OH, MI, IN, WI, IL, and MN and all of MO, IA, SD, ND, NE, and KS

2.2 USEPA National Fish Consumption Rate

USEPA has historically excluded marine fish from the fish consumption rate used to derive its recommended HHWQC. However, the FCR used to derive the 2015 HHWQC incorporates marine species based on the assumption that fish classified as marine but caught in near shore waters represent "local" fish that could be affected by chemicals at a concentration equal to the HHWQC. The key assumption is that near shore waters (within approximately three miles of the shoreline) have concentrations of chemicals equal to the HHWQC (i.e., the maximum allowed in fresh waters) and that the fraction of marine species assumed to be harvested from such near shore waters have spent sufficient time in such waters to have their tissue concentrations in equilibrium with the concentration in the near shore waters, where the equilibrium concentration in fish is defined by the BAF. Neither of these assumptions is likely to be representative of marine fish in near shore waters and, thus, of marine fish harvested from such waters.

As described in more detail in Section 5, below, to the extent near shore waters are affected by concentrations of chemicals regulated by HHWQC, those chemicals are present in such waters because they were discharged in a freshwater environment, transported to the near shore waters by way of a river, and then released into the near shore waters at the mouth of the river. Even if one assumes that the concentration of the chemical in the river water at its mouth prior to release to the ocean is equal to the HHWQC, which is a very unrealistic assumption given that most discharges are diluted by river flow, the concentration in the near shore waters will be greatly diluted by the volume of the ocean, tidal exchange, and ocean currents. The concentration of chemicals in near shore waters as defined by USEPA will be lower than HHWQC and, therefore, also lower in marine fish caught from such waters than assumed by the 2015 HHWQC. Indeed, the concentrations may be so much lower as to not to lead to a material increase in exposure. Moreover, concentrations of many chemicals in mussels and oysters collected from near shore waters have been decreasing over the past two decades or more (O'Conner and Lauenstein 2006), raising the question of why the list of fish species included in the FCRs used to derive the 2015 national HHWQC was expanded to include marine fish.

As described above, the NCI methodology reduces the high bias in the upper percentiles of fish consumption rates from short-term surveys. Given that reduction in bias, use of the NCI methodology might have been expected to result in a decrease in the 90th percentile fish consumption rate of 17.5 g/day used by USEPA to derive the pre-2015 National HHWQC. Inclusion of marine species and some salmon (see next section) may, therefore, explain why the 90th percentile FCR used by USEPA to derive the 2015 National HHWQC increased from 17.5 g/day to 22 g/day. USEPA's lack of transparency regarding species-specific FCRs will create a challenge for States to use the USEPA FCR data and develop FCRs representative of the fish species consumed from a State's waters. However, it bears pointing out that USEPA (2014a) does provide information on the long-term FCR of just freshwater finfish and shellfish (summarized for different regions of the US in Table 2). These freshwater only FCRs are substantially lower than the 90th percentile FCR of 22 g/day used by USEPA that included salmon and some marine fish. They are also more representative of the species of fish that may be consumed by residents of inland states whose waters do not contain estuarine and marine fish.

Table 2. National and Regional Fish Consumption Rate Estimates for Total, Freshwater and Estuarine, and Freshwater Finfish and Shellfish

Population	All Finfish and Shellfish		Freshwater and Estuarine Finfish and Shellfish		Freshwater Finfish and Shellfish	
	Mean (grams/day)	90th Percentile (grams/day)	Mean (grams/day)	90th Percentile (grams/day)	Mean (grams/day)	90th Percentile (grams/day)
National						
National	23.8	52.8	9.2	22.0	4.4	6.7
Region[1]						
Northeast	30.2	65.2	9.7	23.1	1.6	2.8
Midwest	17.6	39.2	6.0	14.3	5.1	7.5
South	23.7	52.1	11.0	26.3	6.5	10.7
West	25.9	55.7	9.5	22.4	2.5	4.0
Coastal Status[2]						
Noncoastal	21.7	48.3	7.9	19.0	4.3	6.5
Coastal	27.5	59.9	11.5	27.1	4.4	7.0
Coastal/Inland Region[3]						
Pacific	28.5	61.2	11.6	27.3	3.0	4.8
Atlantic	31.4	67.2	13.3	30.8	4.7	7.8
Gulf of Mexico	25.2	55.0	12.2	28.6	5.5	9.3
Great Lakes	19.2	41.8	6.9	16.5	5.4	7.4
Inland Northeast	27.9	60.7	8.7	21.0	1.6	2.6
Inland Midwest	17.1	38.3	5.7	13.5	4.9	7.4
Inland South	21.2	46.9	9.5	22.8	6.8	10.9
Inland West	23.7	50.6	7.7	18.2	2.1	3.4

Notes:

Fish consumption rate estimates are total freshwater and estuarine finfish and shellfish usual fish consumption rate estimates, raw weight, edible portion, for adults.

1. U.S. Census Regions
   Midwest = OH, MI, IN, WI, IL, MO, IA, MN, SD, ND, NE, and KS
   Northeast = PA, NY, NJ, CT, RI, MA, NH, VT, and ME
   South = DE, MD, DC, VA, WV, KY, TN, NC, SC, GA, AL, MS, FL, LA, AR, OK, and TX
   West = NM, CO, WY, MT, ID, UT, AZ, NV, CA, OR, WA, AK, and HI
2. All counties that bordered the Pacific or Atlantic Oceans, the Gulf of Mexico or any of the Great Lakes were defined as coastal. Additionally, counties that bordered estuaries and bays were defined as coastal as were counties whose centroid was within approximately 25 miles of any coast even if not directly bordering a coast.
3. Coastal and Inland Regions
   Pacific Coast = coastal counties in CA, OR, WA, AK, and HI
   Atlantic Coast = coastal counties in CT, DE, DC, FL (bordering Atlantic Ocean), GA, ME, MD, MA, NH, NJ, NY, NC, PA, RI, SC, and VA
   Gulf of Mexico Coast = coastal counties in AL, FL (bordering Gulf of Mexico), LA, MS, and TX
   Great Lakes Coast = counties bordering the Great Lakes in MI, WI, OH, NY, MN, IN, IL, and PA
   Inland West = remaining counties in CA, OR, WA, AK, and HI and all of NM, CO, WY, MT, ID, UT, AZ, and NV
   Inland South = remaining non-coastal counties in DE, MD, DC, VA, NC, SC, GA, AL, MS, FL, LA, and TX and all of WV, KY, TN, AR, and OK
   Inland Northeast = remaining counties in PA, NY, NJ, CT, RI, MA, NH, and ME and all of VT
   Inland Midwest = remaining counties in OH, MI, IN, WI, IL, and MN and all of MO, IA, SD, ND, NE, and KS

2.3 Inclusion of Anadromous Fish

Unlike true freshwater species, anadromous fish spend a substantial fraction of their life in marine or ocean environments that are outside States' jurisdiction. If a substantial fraction of the chemical-specific body burden (mass per fish) found in returning adult salmon is acquired during time spent in the ocean, there is effectively nothing a State will be able to do to reduce risks to humans resulting from exposure to chemicals in the salmon they eat. For this reason, the FCR of 17.5 g/day used by USEPA to derive HHWQC prior to 2015 classified salmon as a marine fish and excluded salmon[3] from the FCR (USEPA 2000). While USEPA (2014) recognizes that habitat apportionment is complicated by the fact that some species live in multiple habitat types at different life stages, the method used to apportion consumption of anadromous fish to estuarine/near shore and marine habitats is unclear. For example, an apportionment of 15% estuarine and 85% marine is assigned to both chum salmon and coho salmon, with a note simply indicating that "some populations spend many months in estuaries." In the past, USEPA has designated Pacific salmon as marine species, effectively excluding them from the FCR used to derive HHWQC (USEPA 2000, 2002a), as it was commonly accepted that salmon accrue most of their body mass and chemical body burden in marine waters. However, in recent years, the treatment of salmon and other anadromous species in the FCR used to derive HHWQC has been called into question (e.g., WDOE 2013). Not only are salmon of particular cultural significance in the Pacific Northwest, but their life histories are varied and complex. While all current research supports a conclusion that the majority (i.e., >90%) of the bioaccumulative chemical body burden in adult Pacific salmon is acquired in the marine phase of their life (Cullon et al. 2009, O'Neill and West 2009), this has not necessarily been proven for all anadromous fish. Therefore, there is some debate about the best approach to apportionment for these species. The ultimate question is what fraction of the final chemical burden in a State's returning adult salmon is acquired in the State vs. in the ocean.

It is to be expected that if salmon spend time in both freshwater and saltwater habitats, they will accumulate contaminants in both types of habitats. The scientific literature (e.g., Johnson et al. 2007a,b) shows that juvenile salmon caught in freshwater contain some mass of persistent bioaccumulative toxins (PBT; i.e., chemicals such as PCBs) prior to outmigration to the ocean. However, unless these observations are paired with measurements of PBT burdens in returning adults, the relative significance of the mass accumulated by juveniles in freshwater cannot be assessed. Thus, standalone measurements in juvenile fish are not directly relevant to the central question of where adult salmon accumulate their cumulative PBT body burdens.

A review of the scientific literature shows only a handful of studies providing results relevant to this question, with the work of O'Neill, West, and Hoeman (1998), West and O'Neill (2007), and O'Neill and West (2009) constituting the most thorough examination of the issue. O'Neill and West (2009) found that PCB levels in adult Chinook salmon (fillets) collected from a wide range of geographic locations are relatively uniform except for fish taken from Puget Sound, which show three to five times higher levels of PCBs than fish taken from other locations. As discussed by the authors, these data can be interpreted as indicating accumulation of PCBs in Puget Sound and/or along the migratory routes of these fish, which, depending on the specific runs, can pass through some highly-contaminated Superfund sites (e.g.,

[3] Landlocked and farm-raised salmon were included in the 17.5 g/day FCR, even though they represented a small fraction of total salmon consumed (USEPA 2000).

Duwamish Waterway). Ultimately, however, O'Neill and West (2009) concluded that, on average, greater than 96% of the total body burden (mass) of PCBs in these Puget Sound Chinook was accumulated in the Sound and not in natal river(s) based on a comparison of PCB concentrations and body burdens in out-migrating Chinook smolts collected from the Duwamish River and adults returning to the Duwamish.

Even the most contaminated out-migrating smolts contained no more than 4% of the body burden (mass) of PCBs found in returning adults. Thus, greater than 96% of the PCB mass (burden) found in the returning adults was accumulated in marine or ocean waters (including Puget Sound). Even allowing for an order of magnitude underestimate in the body burden of out-migrating smolts, O'Neill and West (2009) concluded that accumulation in freshwater would account for less than 10% of the average PCB burden ultimately found in adults returning to the Duwamish River. By extension, this analysis supports the conclusion that Chinook salmon passing through uncontaminated estuaries during outmigration accumulate a dominant fraction of their ultimate PCB body burdens in the open ocean. Other researchers have also reached this conclusion using their own data, and Cullon et al. (2009) concluded that 97% to 99% of the body burdens of various PBT chemicals were acquired during the time at sea (based on measurements in out-migrant juvenile and returning adult Chinook from multiple natal rivers).

Overall, measurements support the position that, as a general rule, the predominant fraction of the ultimate PBT burden found in harvested adult salmon, even salmon passing through highly contaminated fresh and estuarine waters during outmigration, is accumulated while in the ocean phase of their life cycle (e.g., Cullon et al. 2009; O'Neill and West 2009). This conclusion is supported by modeling as well (Hope 2012). States with near shore waters may want to consider these data when determining how, if at all, to count anadromous fish in the calculation of their fish consumption rates.

2.4 Trends in Fish Consumption Rates

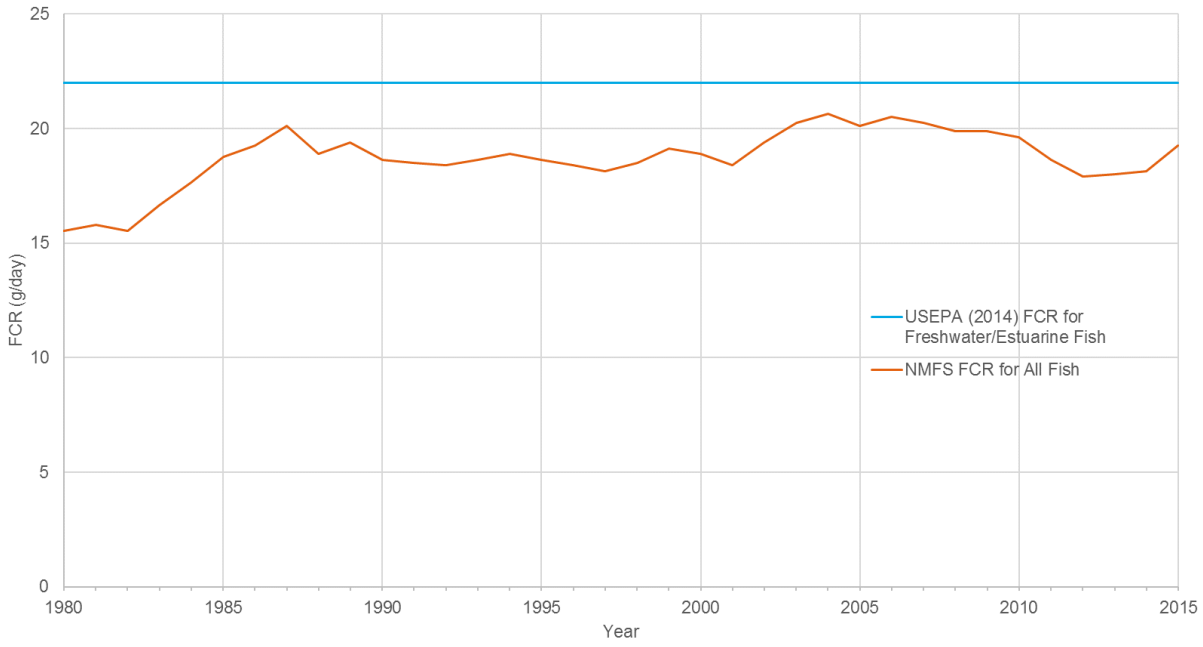
FCRs used by USEPA to derive HHWQC have increased over the years, from 6.5 g/day in 1980 to 17.5 g/day in 2000 and finally 22.0 g/day in 2015 (USEPA 1980, 2000, 2015a). However, the increases in FCRs used by USEPA to derive HHWQC are primarily due to policy decisions (e.g., changes in calculation methodology, change in percentile/statistic of the distribution used to represent fish consumption, and inclusion/exclusion of certain species) and do not reflect a national trend of increasing FCRs over time.

The per capita consumption of all fish and shellfish tracked by the National Marine Fisheries Service (NMFS) has remained essentially unchanged since 1985. NMFS data show only a slight step increase from approximately 15 g/day in the early 1980s to approximately 19 g/day in the mid-1980s (Figure 1). The NMFS calculation of per capita consumption is based on a "disappearance" model. Per NMFS (2016), "The total U.S. supply of imports and landings is converted to edible weight; decreases in supply, such as exports and industrial uses, are subtracted. The remaining total is divided by the U.S. population to estimate per capita consumption." Because the NMFS fish consumption rates include data for all freshwater, estuarine, and marine species, the per capita rate of about 19 g/day is higher than the national average FCR estimated by USEPA of 9.2 g/day (Tables 1 and 2) which does not include marine fish. When USEPA includes marine fish, the FCR for all fish and shellfish is 23.8 g/day (USEPA 2014a), similar to the 19 g/day reported by NMFS.

Given the relatively constant consumption rate of fish over the past thirty years, as States consider whether to modify the fish consumption rates they have used when deriving State-specific HHWQC, it is

important that States identify and be transparent about the basis for such modifications. Changes could be based on new science (e.g., new consumption rate surveys, application of the NCI methodology) and/or changes in policy (e.g., inclusion of anadromous and marine species, selection of the population to which the FCR applies, which percentile or other statistical metric to use).

Figure 1. NMFS Fish Consumption Rate Trend



Notes:
National Marine Fisheries Service (NMFS). 2016. Fisheries of the United States, 2015. U.S. Department of Commerce, NOAA Current Fishery Statistics No. 2015. Available at: https://www.st.nmfs.noaa.gov/commercial-fisheries/fus/fus15/index

3 RELATIVE SOURCE CONTRIBUTION

The relative source contribution (RSC) is an explicit parameter in USEPA's derivation of HHWQC. It applies only to HHWQC based on toxicological endpoints with a mode of action assumed to have a threshold (e.g., most non-cancer endpoints, non-linear cancer endpoints). The concept embodied by the RSC is that a person's total exposure to a chemical should not exceed the allowable exposure (i.e., the reference dose [RfD]). Exposure can come from a variety of pathways in addition to drinking of surface water or consumption of fish from waters regulated by HHWQC. The other pathways most frequently mentioned are exposures through inhalation and consumption of food. The RSC is used by USEPA to derive or establish the fraction of the RfD that can be apportioned to exposures from surface water when deriving HHWQC.

3.1 Origins of the RSC

The concept of the RSC has a long history. When developing national drinking water criteria in the mid-1970's as part of a collaboration with USEPA under the Safe Drinking Water Act (SDWA), the National Academy of Sciences (NAS) appears to have been one of the first to recognize that the combination of drinking water exposures regulated by drinking water standards combined with exposures from other sources (e.g., inhalation of air, consumption of food) could cause a person's total exposure to exceed the RfD (NAS 1977):

> *Since the calculation of the [acceptable daily intake (ADI)] values is based on the total amount of a chemical that is ingested, the ADI values calculated in this report do not represent a safe level for drinking water. However, a suggested no-anticipated-adverse-effect level has been calculated for these chemicals in drinking water using two hypothetical exposures (where water constitutes 1% and 20% of the total intake of the agent), and similar calculations can readily be made for other exposures.*

Though the NAS did not refer to the 1% and 20% as an RSC, the percentages serve the same purpose; assuming that either 1% or 20% of the acceptable daily intake (ADI) (the equivalent of the RfD) can be allotted to exposures from drinking water. The remainder (either 99% or 80%) was allotted to other sources of exposure.

Shortly thereafter, in 1980, the RSC concept was included by USEPA in the derivation of surface water quality criteria (USEPA 1980). For surface water quality criteria USEPA proposed to address exposures from other sources by subtracting exposures from diet and inhalation using the equation shown below (USEPA 1980).

$$C = ADI - (DT + IN) / [2\ L + (0.0065\ kg \times R)]$$

Where:

C is the criterion;
ADI is the acceptable daily intake (now called the reference dose (RfD));
2 L is the assumed daily water consumption;
0.0065 kg is the assumed daily fish consumption;
R is the bioconcentration factor (units of liters per kilogram [L/kg]);
DT is the estimated non-fish dietary intake; and
IN is the estimated daily intake by inhalation.

USEPA goes on to state "If estimates of IN and DT cannot be provided from experimental data, an assumption must be made concerning total exposure. It is recognized that either the inability to estimate DT and IN due to lack of data or the wide variability in DT and IN in different states may add an additional element of uncertainty to the criteria formulation process. In terms of scientific validity, the accurate estimate of the Acceptable Daily Intake is the major factor in satisfactory derivation of water quality." (USEPA 1980). Review of the criteria proposed by USEPA in 1980 indicates that for most, if not all compounds, both DT and IN were set to zero. In other words, non-fish dietary exposures and inhalation exposures were assumed to be zero. In 1991, USEPA discussed this assumption more explicitly stating "Where dietary and/or inhalation exposure values are unknown, these factors can be deleted from the above calculation." (USEPA 1991a).

Prior to 2015, HHWQC for most compounds were derived assuming the contribution from non-fish dietary sources and inhalation was assumed to be zero, the equivalent of setting the RSC to 1. The RSC was assumed to be 1 despite USEPA developing an extensive Decision Tree Approach (with 10 pages of supporting discussion) about the use of the RSC when deriving HHWQC (USEPA 2000). That decision tree distinguishes between RSCs derived using the subtraction method and the percentage method[4]. The subtraction method is essentially the same[5] as described in earlier USEPA HHWQC support documents (USEPA 1980, 1991a) and drinking water standard support documents (USEPA 1985, 1989a). What exactly USEPA intended when applying the percentage method is not as clear because, prior to 2000, HHWQC guidance referred to only the subtraction method. However, drinking water standards referred to both the subtraction method and the percentage method (USEPA 1985, 1989a).

In 1985, USEPA proposed national primary drinking water standards that used an RSC when deriving drinking water standards, though it was not yet referred to as the RSC at that time (USEPA 1985). In that proposal, USEPA describes two different approaches for deriving the equivalent of RSCs. When sufficient data about the magnitude of other sources of exposure are available, the drinking water standard is set by subtracting the exposure from other sources (e.g., air and food) from the RfD. This is referred to as the subtraction method. It is essentially the same as the subtraction method referred to by the USEPA (1980) for deriving HHWQC differing only in structure of the equations used to derive the standards/criteria. When sufficient data on exposure from sources other than drinking water are not available, USEPA proposes deriving the drinking water standard by multiplying the RfD by the assumed percentage of the RfD that is contributed by drinking water (USEPA 1985). This is referred to as the percentage method.

USEPA (1985) also establishes 20% as the assumed contribution of drinking water to allowable exposure when comprehensive data on exposure from other sources are not available. USEPA states that “this exposure factor is judgmental and is adjusted when mitigating information exists” and that “use of a 20% contribution is considered to be reasonably conservative.” Four years later, USEPA also established a maximum RSC of 80% (USEPA 1989a). USEPA states “If data indicate that drinking water is responsible for a large part of total exposure to a chemical (i.e., 80 to 100 percent), EPA believes that it is prudent to allow for the contingency that exposure via air, food and other sources that may not be reflected in the available data is likely to occur. Utilizing the 80% “ceiling” for drinking water exposures ensures that the maximum contaminant level goal (MCLG) will be low enough to provide adequate protection for individuals whose total exposure to a contaminant is, due to dietary or other exposure, higher than currently indicated by available data. This approach, in effect, introduces an additional uncertainty factor…it ensures that the MCLG will result in no adverse effect with an adequate margin of safety.” (USEPA 1989a).

When describing the subtraction and percentage methods, USEPA suggests that data about the magnitude of sources of exposure other than drinking water are likely available for inorganic compounds and are unlikely to be available for many organic compounds (USEPA 1985, 1989a).

[4] In the subtraction method, the exposure supported by the RfD is allocated among various sources by first subtracting all exposure routes other than drinking water and fish consumption and then allocating the remainder of the RfD to drinking water and fish consumption. The percentage method is a simple ratio of exposure via drinking water and fish consumption to the total exposure.

[5] The equation is slightly different but the concept of reducing the portion of the RfD available for deriving HHWQC based on non-fish dietary and inhalation exposures is the same.

3.2 RSC Decision Tree

A detailed discussion of the application of the subtraction and percentage methods when developing HHWQC is provided in USEPA (2000). That discussion includes a recommended Decision Tree Approach for when each method is applicable. The scientific and policy basis for several of the decision points in the Decision Tree are worthy of more detailed consideration to determine whether the approach is applicable and relevant to individual States.

- The description of the subtraction approach is consistent with descriptions in prior USEPA guidance (USEPA 1980, 1985, 1989a, 1991a). However, the description of the percentage approach differs from previous descriptions presented in drinking water standard guidance (USEPA 1985, 1989a). When describing the percentage approach in 1989, USEPA states "When data did not exist, EPA then estimated drinking water's contribution at 20 percent of total exposure." (USEPA 1989a). In other words, when USEPA did not have information on the magnitude of exposure from other sources, it selected 20% as the default RSC. The description of the percentage method in USEPA (2000) assumes information about other sources is available. The percentage method is described as "This simply refers to the percentage of overall exposure contributed by an individual exposure source. For example, if for a particular chemical, drinking water were to represent half of total exposure and diet were to present the other half, then the drinking water contribution (or RSC) would be 50 percent." (USEPA 2000). This definition assumes information about total exposure is available. The presumption that information on total exposure is available is further reinforced by a recent description of the percentage method (USEPA 2015b, see Attachment C). Previous descriptions of the percentage method state the method is to be used when information on other exposure sources is absent. If total exposure can be quantified, then information on other sources must be available. If such information is available and is reliable enough to develop an estimate of total exposure, then the percentage method (at least as described prior to 2000) would not need to be used to estimate an RSC.
- Given the descriptions in the 2000 HHWQC guidance, the health protection achieved by the two alternative approaches to the percentage method differ. In the approach used to establish drinking water standards, where the contribution of drinking water to the RfD is simply set at a specific percentage, drinking water exposures can be as high as the set percentage, but will not exceed that percentage. As long as that percentage is less than 100% (i.e., the RSC is less than 1), drinking water exposures will not exceed the RfD. And as long as exposure from other sources is no more than the 80% of the RfD, total exposure will not exceed the RfD. In the approach described by USEPA (2000) where the RSC is determined by the percentage that surface water exposures represent of total exposure, relatively small surface water exposures will remain small. However, relatively large drinking water exposures will remain large (see Attachment C). As long as total exposure is less than the RfD, exposures from surface water will also be less than the RfD. However, it is possible for this application of the percentage method to result in total exposures that exceed the RfD. One example is a situation where total exposure is equal to the RfD, surface water exposures are a relatively large proportion of that total exposure and new toxicity data become available that lead to a decrease in the RfD such that the existing total exposure now exceeds the new RfD. Because the percentage that surface water comprises of total exposure remains the same (exposures did not change, only the RfD), the RSC remains

the same and can result in a situation where total exposure exceeds the RfD (see Attachment C). This is an example of where the percentage method would not meet the stated goal of using a RSC "…the purpose of the RSC is to ensure that the level of chemical allowed by a criterion or multiple criteria…will not result in exposure that exceed the RfD…" (USEPA 2000). States should recognize that unlike the subtraction method, the percentage may not meet the fundamental goal of the RSC under certain conditions.

- The Decision Tree Approach indicates that the subtraction method should not be used for compounds that have criteria or standards for other environmental media. That distinction was not raised when the two methods were discussed in drinking water standards guidance (USEPA 1985,1989a). Nor is it clear why the distinction is being made in the 2000 HHWQC guidance. USEPA states "When more than one criterion is relevant to a particular chemical, apportioning the RfD…via the percentage method is considered appropriate to ensure that the combination of health criteria, and thus the potential for resulting exposures, do not exceed the RfD…" (USEPA 2000). That statement fails to explain how applying the percentage method to HHWQC would keep total exposure from exceeding the RfD. The RSC is only applied to surface water criteria or drinking water standards. Apportioning the RfD in only one medium (e.g., surface water or drinking water) and not the others (e.g., air, foodstuffs) can still lead to the potential for total exposure to exceed the RfD. Each medium for which standards/criteria are based on an unapportioned RfD could by themselves have exposures equal to the RfD. When all exposures are combined, the RfD could be exceeded. Such an interpretation also assumes that concentrations in all environmental media are always equal to applicable criteria/standards. Given that criteria/standards are often enforced in a manner that leads to media concentrations well below concentrations allowed by criteria/standards (see Attachment G), the assumption that media concentrations will always be equal to the criteria/standards adds another uncertainty factor that may not be necessary. If data for the chemical in environmental media indicate that concentrations are lower than allowed by criteria/standards and are expected to remain that way, States should consider whether it is reasonable and necessary to use the more recent 2000 description of the percentage method and effectively assume concentrations are equal to criteria/standards, particularly if the enforcement methodology will continue to preclude such concentrations.
- The Decision Tree Approach also recommends evaluation of data adequacy and sufficiency. The associated discussion describes quite rigorous thresholds for data adequacy, though it does start out by recognizing application of professional judgment (USEPA 2000). Whether it represents professional judgment on USEPA's part or some alternative decision process to arrive at RSCs, it is important for States to recognize that some of the existing RSCs that differ from USEPA's default floor of 0.2 were derived prior to publication of the Decision Tree Approach and are unlikely to be consistent with all the data thresholds described therein. For example, when setting drinking water standards, USEPA uses a RSC of 0.8 for barium (USEPA 2016a). That RSC was derived by USEPA in 1985 (USEPA 1985). In that derivation, USEPA states "Little data are available on the level of barium in the U.S. food supply...Studies of four individuals indicated the dietary intake of barium ranged from 440 to 1,800 ug/day. The "average" value of 900 ug/day reportedly includes intake from beverages. The ICRP reports an "average" daily dietary intake of 750 ug/day for an adult male from food and fluids, of which 80 ug/day comes from drinking water. Based on these data, the diet contributes approximately 670 ug barium to the adult human intake

each day." (USEPA 1985). USEPA then goes on to use that estimate of exposure to derive the RSC of 0.8 for barium that is still used today. USEPA also uses a RSC of 0.4 when deriving the HHWQC and MCLG for antimony (USEPA 2002b, 1992). That RSC was derived in 1992 and is based on a survey of antimony in drinking water and a Food and Drug Administration (FDA) study of contaminants in food. Review of these studies should provide States a sense of the data requirements USEPA relies upon for HHWQC RSCs and the kind of deviations from data adequacy thresholds in the Decision Tree Approach that USEPA may find acceptable when deriving State-specific RSCs.

Note as well that inclusion of salmon in the FCR (discussed above in Sections 2.1 and 2.2) can lead to a "double counting" of potential exposure to a compound in the derivation of HHWQC if the RSC is used to account for exposures from consumption of fish such as salmon that accumulated their body burden of a compound while in the marine environment. The goal of the RSC is to account for exposures not affected by HHWQC. Including salmon increases the FCR and reduces the HHWQC. The potential exposure from consumption of salmon is accounted for by such inclusion. However, if HHWQC are further reduced through the application of a RSC to account for exposures of salmon in the marine environment, then the HHWQC is reduced further. That further reduction is not necessary because the exposure from such salmon was already addressed by the inclusion of salmon in the FCR used to derive the HHWQC. Such double counting can be prevented by either not including salmon in the FCR or not including exposures associated with consumption of salmon in the RSC.

3.3 Application of RSCs

When using RSCs to derive state-wide criteria, States should appreciate and carefully consider at least five points.

First, are RSCs needed at all? The concept embodied by the RSC was recognized by USEPA in 1980, but it was not until 2015, 35 years later, that USEPA included an RSC of less than 1 when deriving HHWQC for most compounds. USEPA has referred to these as an "additional uncertainty factor." As discussed in other sections of this document and attachments, numerous conservative assumptions are already used to estimate exposure and toxicity when deriving HHWQC. Is another one necessary? Have data come to light in those intervening 35 years to suggest that exposures from other sources have been increasing or are larger than USEPA and States have been assuming for the past 35 years and, therefore, is application of an RSC and an added uncertainty factor to account for such exposures necessary?

Second, if an RSC is needed, should it be developed using the subtraction or percentage method? The Decision Tree Approach in USEPA (2000) sets forth a series of conditions that lead to selection of one approach over the other. The basis for some of those conditions is unclear (such as the recommendation to use the percentage method if the compound is regulated in other environmental media) and should be carefully considered and the applicability to a particular State understood before deciding upon the method. Additionally, as noted above, under certain conditions, the percentage method may not meet the original goal of the RSC; to assure the total exposure from all sources remains below the RfD. Finally, USEPA also points out that situations may exist where the decision tree "is not practicable or may simply be irrelevant after considering the properties, uses, and sources of the chemical in question" and goes on to state "EPA endorses such flexibility…to choose other procedures that are more appropriate for setting

health-based criteria and, perhaps, apportioning the RfD…as long as reasons are given as to why it is not appropriate to follow the Exposure Decision Tree approach and as long as the steps taken to evaluate the potential sources and levels of exposure are clearly described." (USEPA 2000).

Third, regardless whether the percentage or subtraction method is used to derive an RSC, should the default of 20% used by USEPA for most compounds be employed? As noted above under the first consideration, many more data are available now than were available 30 years ago on the potential exposure to many of the compounds for which HHWQC may be proposed. These data may indicate that exposures from other sources are lower than assumed by a default RSC of 20% (i.e., sources other than surface water contribute less than 80% of the RfD) and that a data-derived RSC is scientifically defensible and appropriate. Examples of such RSCs are provided in Attachment D.

Fourth, when deriving a State-specific RSC, must the data requirements set forth in USEPA (2000) be adhered to, or is the totality of data that have been collected on environmental concentrations of compounds in the past three decades (since USEPA [1985] raised the data-based distinction between the subtraction and percentage methods) sufficient to make well-informed assessments of exposure from the diet and air? USEPA (2000) contains rather extensive requirements for data to be considered usable when deriving a State-specific RSC. However, review of the data used by USEPA to derive RSCs for some drinking water standards, and in a few instances for HHWQC, suggests that those same data quality thresholds would not be met by several of the current RSCs that differ from the default of 20%. USEPA (2000) does note that a "case-by-case determination may be necessary" and that "data may, therefore, be adequate for some decisions and inadequate for others; this determination require some professional judgment (USEPA 2000).

Fifth, if a default RSC is determined to be appropriate, should USEPA's uniform range of default RSCs of 20% to 80% be used for all compounds? The original default floor and ceiling of 20% and 80%, respectively, were developed for drinking water standards, not surface water quality criteria (USEPA 1989a). Surface water quality criteria include both drinking water and dietary (fish consumption) exposure pathways. In other words, a portion of the dietary exposure accounted for the by the default RSC range of 20% to 80% used to establish drinking water standards is regulated by HHWQC. For bioaccumulative compounds, the portion of a person's total dietary exposure regulated by HHWQC may be quite large if high fish consumption rates are used to derive HHWQC[6]. States should consider whether the default RSCs developed for drinking water only exposures are applicable to HHWQC developed to regulate exposures from ingestion of surface water and consumption of fish from surface water.

[6] Consider a simple example using the subtraction method where the total exposure is known and that exposure and the allowable exposure are both 100 milligrams per day (mg/day). Further, assume that drinking water contributes 25 mg/day, consumption of fish contributes 50 mg/day and consumption of other dietary items contributes 25 mg/day. The compound is not present in air. Therefore, inhalation does not contribute to total exposure. The amount of the RfD available for drinking water exposure is 25 mg/day (RfD – total dietary intake – inhalation; 100 – 75 – 0 = 25 mg/day) equivalent to an RSC of 0.25. The RSC for surface water exposure that includes exposures through ingestion of water and consumption of fish will be different. The portion of the dietary intake comprised of fish is regulated by the criterion and should not be subtracted from the RfD. For surface water, the amount of the RfD available for drinking water ingestion and fish consumption is 75 mg/day (RfD – non-fish dietary intake – inhalation; 100 – 25 – 0 = 75 mg/day) equivalent to a RSC of 0.75. This is a simple example pointing to what seems a common-sense realization that the default RSC for criteria regulating only one pathway (drinking water) should be different from the default RSC for criteria regulating multiple pathways (drinking water and fish consumption).

4 BIOCONCENTRATION AND BIOACCUMULATION FACTORS

Estimating bioaccumulation of substances from ambient surface water into fish is a critical component in USEPA's derivation of HHWQC. USEPA's Technical Support Document, Volume 2 (USEPA 2003) defines bioaccumulation as "the uptake and retention of a chemical by an aquatic organism from all surrounding media (e.g., water, food, sediment)" and bioconcentration as "the uptake and retention of a chemical by an aquatic organism from water only". USEPA's (2000) Human Health Methodology gives preference to BAFs over bioconcentration factors (BCFs) because a BAF considers the potential chemical accumulation from all exposure pathways, not just water. However, relative to BCFs, which are typically derived in controlled laboratory studies, measured BAFs are rare and more difficult to estimate owing to the added complexity associated with the influence of food sources, sediment factors, and variable ambient conditions. Thus, USEPA's 2000 Human Health Methodology includes use of BCFs to estimate BAFs for criteria derivation. When USEPA updated its national HHWQC in 2015, a key change was using BAFs instead of BCFs to predict the uptake of substances by fish from surface water.

This section provides States and other stakeholders with two important pieces of information. First it provides an overview of the key aspects of the procedures USEPA followed to derive national BAFs used in the development of the 2015 national HHWQC. Second, it illustrates alternative procedures that can be used by States to develop BAFs that are more appropriate and that reflect ambient conditions more closely linked to those that exist outside of the Great Lakes.

For most substances[7], the USEPA methodology involves estimating a baseline BAF (i.e., a BAF based on the dissolved fraction and adjusted for lipid concentration) based on field or laboratory studies if available. When measured BAFs are available USEPA's procedure uses those to estimate bioaccumulation. When measured BAFs are not available USEPA estimates BAFs by multiplying either measured or modeled BCFs by a foodchain multiplier (FCM). The FCM is intended to account for exposure of fish and shellfish from the non-water exposure pathways. A detailed discussion of the derivation and application of FCMs is presented in Attachment L. Exceptions to this process include inorganic compounds that are not expected to biomagnify, ionized organic compounds, organic compounds with log K_{ow} of less than 4, and organic compounds that are highly metabolized. For compounds that fall into any of these four categories, USEPA's procedure suggests using a field measured BAF and, if such is not available, a laboratory derived BCF.

Many BAFs used by USEPA for derivation of the 2015 HHWQC were developed from data for polychlorinated biphenyls (PCBs) in the Great Lakes. As described in Attachment L, incorporation of assumptions that might be more representative of surface waters outside of the Great Lakes requires developing alternative inputs and running a bioaccumulation model. Recognizing that not all States will have the resources, expertise, or time, to become familiar with and run the model, alternative sets of FCMs are developed in Attachment L. The different sets capture the FCMs for substances that have metabolic transformation rates that differ from PCBs and surface waters that have foodwebs and characteristics (e.g., temperature, sediment-water ratio) that differ from the Great Lakes. This information

[7] BCFs, and not BAFs, were developed and used to derive the proposed HHWQC for some substances.

should allow States to select and apply FCMs to the derivation of BAFs that are more applicable and representative of surface waters in their States without having to run the bioaccumulation model.

Attachment L describes USEPA's BAF derivation in substantial detail with the goal of allowing interested States to develop alternative, State-specific BAFs for several of the substances USEPA considers bioaccumulative. The remainder of this section provides brief summaries of the key technical issues discussed in more detail in the three attachments referred to below.

4.1 Development of State-Specific FCMs and BAFs

USEPA's BAF methodology specifically allows for the conversion of USEPA's default National BAFs to State-specific BAFs using State-specific assumptions about the concentration of dissolved organic carbon (DOC) and particulate organic carbon (POC) in surface water, parameters used to calculate the freely dissolved fraction in surface. USEPA's methodology also allows the incorporation of State-specific assumptions for the lipid content of fish and shellfish in each trophic level. A more thorough evaluation of these aspects of the USEPA methodology as it was applied by FDEP when developing Florida-specific HHWQC is included in Attachment E.

Review of the applicability of national FCMs and resulting BAFs indicated that several of the other default assumptions used by USEPA to derive national FCMs are unlikely to be representative of many chemicals and State-specific conditions. Recognizing that not all States will have the resources, expertise, or time, to run the model USEPA used to derive national BAFs, alternative sets of FCMs are developed in Attachment L that account for various combinations of conditions that represent the range of surface water conditions in the United State better than do USEPA's defaults. The different sets of FCMs account for substances that have metabolic transformation rates that differ from PCBs and surface waters that have foodwebs and characteristics (e.g., temperature, sediment-water ratio) that differ from the Great Lakes. This information should allow States to select and apply FCMs to the derivation of BAFs that are more applicable and representative of surface waters in their States without having to run USEPA's bioaccumulation model. The four parameters that are varied to develop the different sets of FCMs in Attachment L (foodweb structure, sediment-water ratio, metabolic transformation rate, temperature) are briefly described below.

First, the model used by USEPA to derive national FCMs is based on and calibrated for a Great Lakes foodweb using PCB data. A State-specific foodweb may have substantially different inputs and structure and could result in different FCMs. As an example, Florida waters do not support alewives, smelt, or salmonids and the lipid content of many fresh water species appears to be lower in Florida than in the Great Lakes (Attachment E). Given the existence of a variety of foodwebs throughout the United States, the methodology presented in Attachment L presents FCMs for three different foodwebs (Great Lakes, warmwater benthic, warmwater pelagic) allowing States to develop refined State-specific FCMs and BAFs more representative of the conditions in their surface waters than those assumed by USEPA's national default BAFs.

Second, USEPA's model assumes that surface waters have had a long history of loading of substances followed by a relatively recent reduction in such loading (such as PCBs in the Great Lakes and Hudson River in the 1980's and 1990's). That scenario of high historic loading leads to a high proportion of a substances in sediments compared to conditions closer to equilibrium. The effect of that model assumption is to increase FCMs. FCMs decrease substantially when substance loading expected to be

representative of most waters in the United States are employed in USEPA's FCM model. The methodology presented in Attachment L presents FCMs for three different sediment-water ratios (23, 10, and 2) allowing States to develop refined State-specific FCMs and BAFs more representative of the conditions in their surface waters than those assumed by USEPA's national default BAFs.

Third, USEPA uses FCMs developed using the assumption of no metabolic transformation to derive HHWQC for many substances that are likely to be metabolized to some degree by fish or shellfish or both. The potential effect on FCMs of incorporating metabolism was previously investigated for pentachlorophenol, heptachlor, and 1,3-dichlorobenzene in Florida waters (Attachment E). When the substance-specific metabolic transformation rate constants were incorporated into the FCM model, the FCMs dropped substantially for all three chemicals (Attachment E). Given the large effect of metabolism seen for the above three substances, the methodology in Attachment L presents FCMs for four different metabolic transformation rates (0, 0.001, 0.01, and 0.1 day^{-1}) that States can use to develop refined substance-specific FCMs and BAFs that account for metabolism.

Fourth, the temperature used in the USEPA model is cooler than might occur in State-specific waters. Use of a higher temperature in the FCM model can increase FCMs because the higher temperature results in an increase in dietary intake in the model. Because the model assumes no metabolic transformation, the increased dietary intake is not balanced by what one might expect to be an increased rate of metabolic transformation as temperature increases. As with foodweb structure, sediment-water ratio, and metabolic transformation described above, the methodology presented in Attachment L presents FCMs for two different temperatures (8° and 16° C) thereby allowing States to develop refined State-specific FCMs and BAFs more representative of the conditions in their surface waters than those assumed by USEPA's national default BAFs.

4.2 Other Technical Issues Associated with USEPA's Application of the BAF Methodology

For bioaccumulative substances that do not have measured BAFs, a key step of USEPA's process for deriving a baseline BAF is multiplying a BCF by a FCM. As noted above, USEPA's guidance lists certain characteristics of a substance that preclude the application of a FCM. One of those characteristics is "high metabolism", which is how USEPA classified polycyclic aromatic hydrocarbons (PAHs). However, for PAHs, USEPA failed to correctly account for high metabolic transformation rates and multiplied laboratory BCFs by FCMs, which is not consistent with its guidance for highly metabolized compounds. Attachment F provides a review of USEPA's application of the methodology when deriving National BAFs for the 12 PAHs for which USEPA updated HHWQC in 2015.

The USEPA database includes invertebrate species (e.g., the water flea (*Daphnia magna*), an amphipod (*Pontoporeia hoyi*), and a mayfly (*Hexagenia limbata*)) that are not representative of shellfish consumed by the general population. Whether the accumulation of substances in typically consumed shellfish is well represented by BAFs and BCFs from amphipods, mayflies and water fleas is unknown. What is known is that these organisms are very different from those that are regularly consumed. Until it has been shown that their BAFs and BCFs are representative of regularly consumed species, States should consider whether it might be best to exclude them when estimating the BAFs and BCFs of regularly consumed shellfish species, particularly for substances for which such species have a strong influence on the Baseline BAF.

USEPA's methodology requires BAFs for each of three trophic levels (trophic levels 2, 3 and 4). When bioaccumulation data specific to each trophic level are available, national trophic level-specific BAFs are developed by USEPA and applied only to the trophic level from which each BAF was derived. For some substances, data to develop national BAFs were available for only one or two trophic levels. When a trophic level-specific BAF could be developed for only one trophic level, that BAF was applied to all three trophic levels. When trophic level-specific BAFs were available for two trophic levels, USEPA applied the geometric mean BAF of those two BAFs to all three trophic levels. Depending upon trophic level and a substance's metabolic transformation rate, application of BAFs across trophic levels can lead to an under- or over-estimate of bioaccumulation. For example, applying a trophic level 2 BAF two all three trophic levels for a substance that undergoes metabolic transformation will overestimate the BAF for trophic levels 2 and 3. However, in that same situation, if the substance undergoes little metabolic transformation, the BAF for trophic levels 3 and 4 will be underestimated.

5 CHEMICAL CONCENTRATION IN RECEIVING WATER

The derivation of the HHWQC assumes that all species included in the FCR are continuously exposed to water that has a chemical concentration equal to the HHWQC. As noted above, the fish consumption rate used to derive the 2015 HHWQC includes not only freshwater and estuarine species, just as have earlier national HHWQC, but also marine species that spend some portion of their time in near-shore waters. For several reasons, the assumption that surface water has a concentration of chemicals equal to HHWQC is unlikely to be true for freshwater and is even less likely to be true for estuarine and near shore waters for several reasons.

Typical regulatory requirements obligate discharges to achieve water quality criteria in the vicinity of the discharge and discharges operate at levels sufficiently below required levels to provide a margin of safety with respect to permit limits based on those criteria. In turn, that means the concentration at the compliance point, likely the edge of the mixing zone (assuming such is allowed), will be less than the HHWQC. How much less will vary depending upon the nature of the receiving water and characteristics of the discharge. Further, because mixing zones are limited in extent, additional dilution occurs outside of the mixing zone before chemicals reach an estuary or near shore waters.

Once a discharge reaches an estuary or near shore waters, dilution will occur based just on volume because of the volume of saltwater compared to freshwater inputs. Beyond volume, additional mixing occurs because of tides, wind driven currents, and currents associated with larger oceanic circulation. Attachment G uses data on salinity for Florida rivers and the estuaries to which rivers discharge to estimate that the standard default assumption of all surface water being equal to the HHWQC overestimates exposure from fish consumption by between 30% to nearly 50%. This estimate is not specific to any single species included in the FCR employed by FDEP to derive HHWQC. It applies to the composite of species included in the FDEP FCR, which means it includes freshwater species. Such species are assumed to be in equilibrium with surface water at the HHWQC and comprised only about 30% (6.7 g/day, Table 2) of the 22 g/day FCR used by USEPA to derive the 2015 National HHWQC. It also includes estuarine and marine species that are assumed to be in equilibrium with chemical concentrations in estuarine and near shore waters. Such waters are assumed to have a chemical concentration less than the HHWQC based on the salinity-based dilution model presented in Attachment G.

When setting State-specific HHWQC, States should consider whether and how to account for the overestimation of exposure and risk associated with the implicit assumption of all waters having chemical concentrations equal to the HHWQC. It can simply be viewed and acknowledged as an additional safety factor that ameliorates in part the need to use conservative values for some of the other inputs to the equation used to set HHWQC. Alternatively, the assumption could be explicitly accounted for by including an input parameter regarding assumed receiving water dilution in the equation used to derive HHWQC.

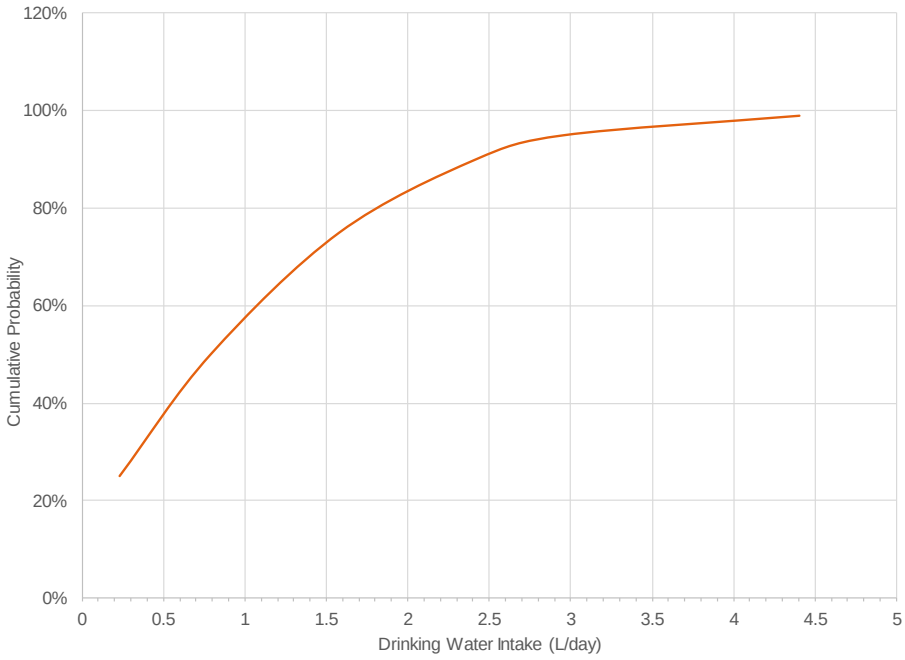
6 OTHER ASSUMPTIONS AND PARAMETERS

Several other exposure parameters are also explicitly included in the equation used to derive HHWQC, including drinking water intake and bodyweight. (As noted above in the introduction, the equation used to derive HHWQC also includes parameters that describe the toxicity of a chemical. This report does not discuss the basis and background of toxicity parameters.) USEPA has established default values to use for these explicit exposure parameters that are generally accepted and used to derive HHWQC as well as other criteria and standards.

6.1 Drinking Water Ingestion

The default drinking water intake is 2.4 liters per day (L/day), representing the per capita estimate of community water ingestion at the 90th percentile for adults ages 21 and older based on National Health and Nutrition Examination Survey (NHANES) data from 2003 to 2006 (USEPA 2015a). Prior to 2015, National HHWQC used a drinking water intake of 2 L/day, which represented the per capita community water ingestion rate at the 86th percentile for adults surveyed in the United States Department of Agriculture's 1994-1996 Continuing Survey of Food Intake by Individuals (CSFII) analysis and the 88th percentile of adults in the National Cancer Institute study of the 1977-1978 Nationwide Food Consumption Survey (USEPA 2015a). The full distribution of drinking water intakes is presented in Figure 2.

Figure 2. Drinking Water Intake Distribution



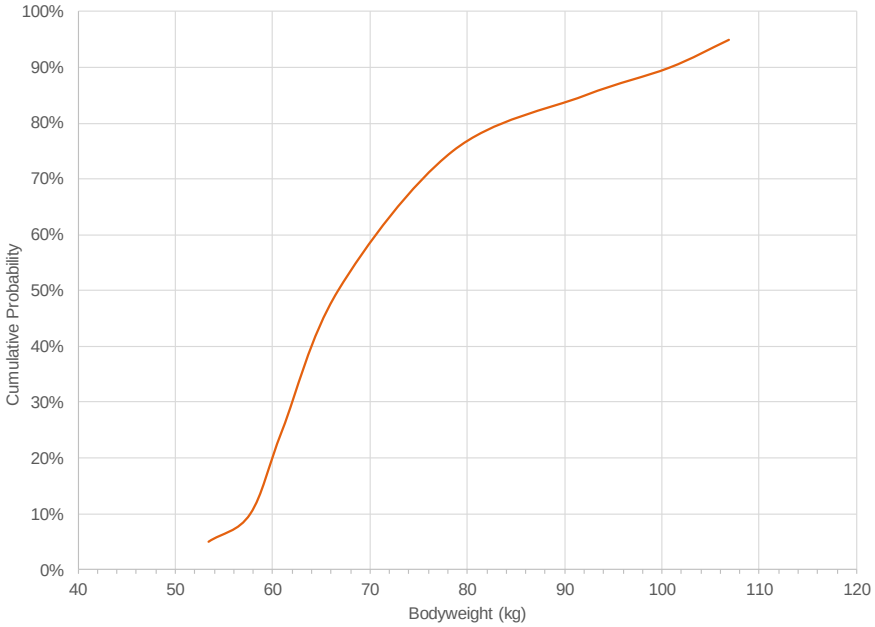
Percentile	Intake (L/day)
Mean	1.043
25%	0.227
50%	0.787
75%	1.577
90%	2.414
95%	2.958
99%	4.405

Notes:
Drinking water intake distribution based on per capita estimates of combined direct and indirect community water ingestion based on NHANES 2003–2006 (USEPA 2011).
USEPA. 2011. Exposure Factors Handbook: 2011 Edition. EPA/600/R-090/052F. Office of Research and Development, Washington, DC.

6.2 Bodyweight

The default bodyweight is 80 kilograms (kg), representing the mean bodyweight for adults ages 21 and older, based on NHANES data from 1999 to 2006 (USEPA 2015a). Prior to 2015, National HHWQC used a bodyweight of 70 kg, which was based on the mean body weight of adults from the NHANES III database (1988-1994) (USEPA 2015a). The full distribution of bodyweights is presented in Figure 3.

Figure 3. Bodyweight Distribution



Percentile	Bodyweight (kg)
Mean	80
5%	53
10%	58
25%	61
50%	67
75%	78
85%	92
90%	101
95%	107

Notes:
Bodyweight distribution derived from NHANES (1999−2006) for adult males and females combined (USEPA 2011).
USEPA. 2011. Exposure Factors Handbook: 2011 Edition. EPA/600/R-090/052F. Office of Research and Development, Washington, DC.

6.3 Other Implicit Assumptions

In addition to the explicit parameters that are the focus of this report, the process used to derive HHWQC makes implicit assumptions about exposure and risk. One such implicit assumption, discussed above, is that the concentration of chemicals in all surface water is equal to the HHWQC. Another implicit assumption mentioned above, is that all fish included in the FCR used to derive the HHWQC have concentrations that are in equilibrium with such surface water concentrations (i.e., fish spend their entire life in surface water with a concentration equal to the HHWQC). Several other implicit assumptions are present as well including the assumption that the concentration of a chemical in fish is not affected (i.e., does decrease or increase) by cooking and other aspects of preparing fish. Available data suggest that some bioaccumulative compounds are lost during cooking (see discussion in Attachments H and I). HHWQC also assume that people effectively use untreated surface water as a drinking water supply because the HHWQC equation contains no explicit parameter to account for any removal of a compound that might occur as a result of treatment by a drinking water supply.

For a more complete list and discussion of implicit exposure assumptions inherent in the HHWQC derivation process see Attachments H and I.

7 COMPOUNDED CONSERVATISM

To date, national HHWQC have been established using predominantly upper bound or maximum values for variables that govern human exposure and toxicity of the compounds that are being regulated. Bogen (1994) pointed out that “safety or conservatism initially assumed for each risk component may typically magnify, potentially quite dramatically, the resultant safety level of a corresponding final risk prediction based on upper-bound inputs.” Collectively, using multiple conservative assumptions results in HHWQC that may be far more protective than necessary to meet risk management goal(s) used to derive the HHWQC. This phenomenon of greater conservatism embodied by the whole than the conservatism of each individual part is referred to as "compounded conservatism" (Nichols and Zeckauser 1986). In the HHWQC derivation process, compounded conservatism plays a role both in the determination of individual factors of the derivation equations (i.e., in the toxicity factors and explicit and implicit exposure elements) and in the equations’ use of multiple factors, each based on upper bound limits and/or conservative assumptions.

In addition to the conservatism embodied in the selection of individual components of the calculations (both explicit and implicit), the fundamental underlying assumption, which is that the most sensitive subpopulations will be exposed to maximum allowable concentrations over a full lifetime, is a highly unlikely and highly protective scenario. For example, the derivation of HHWQC is based on the assumptions that an individual will live in the same place for their entire life (70 years) and that 100% of the drinking water will be untreated and that all of the locally caught fish during those 70 years will come from the local water body, and that local water body will contain regulated substances at the HHWQC concentrations 100% of the time.

The suggestion that the use of multiple default factors based on upper bound limits and/or conservative assumptions lead to a situation of compounded conservatism has been the subject of considerable discussion. However, in a staff paper, USEPA suggests that “when exposure data or probabilistic simulations are not available, an exposure estimate that lies between the 90th percentile and the maximum exposure in the exposed population [should] be constructed by using maximum or near-maximum values for one or more of the most sensitive variables, leaving others at their mean values” (USEPA 2004). This appears to be an acknowledgement that adequately protective assessments do not require that each, or even most, component parameter(s) be represented by a 90th or 95th percentile (or maximum) value.

Similarly, in the 2005 Cancer Risk Assessment Guidelines, USEPA (2005) stated:

> *Overly conservative assumptions, when combined, can lead to unrealistic estimates of risk. This means that when constructing estimates from a series of factors (e.g., emissions, exposure, and unit risk estimates) not all factors should be set to values that maximize exposure, dose, or effect, since this will almost always lead to an estimate that is above the 99th-percentile confidence level and may be of limited use to decision makers.*

Viscusi et al. (1997) provided a simple example to illustrate compounded conservatism. In Superfund exposure assessments, USEPA states that they consider “reasonable worst case” exposures to be in the 90th to 95th percentile range (Viscusi et al. 1997). However, the use of just three conservative default variables (i.e., 95th percentile values) yields a reasonable worst-case exposure in the 99.78th percentile. Adding a fourth default variable increases the estimate to the 99.95th percentile value. In a survey of 141

Superfund sites, the authors reported that the use of conservative risk assessment parameters in site assessments yields estimated risks that are 27 times greater than those estimated using mean values for contaminant concentrations, exposure durations, and ingestion rates.

In a recent report on the economics of health risk assessment, Lichtenberg (2010) noted that the use of conservative default parameters is intended to deliberately introduce an upward bias into estimates of risk. Lichtenberg (2010) also stated that "the numbers generated by such procedures can't really be thought of as estimates of risk, since they bear only a tenuous relationship to the probability that individuals will experience adverse health consequences or to the expected prevalence of adverse health consequences in the population." Indeed, he pointed out that the number of actual cancer deaths that can be attributed to all environmental and occupational causes is much lower than the number that is predicted by risk assessments (Doll and Peto 1981, as cited by Lichtenberg 2010). Lichtenberg (2010) describes concerns about compounded conservatism by saying:

> *...regulators continue to patch together risk estimates using a mix of "conservative" estimates and default values of key parameters in the risk generation process. Such approaches give rise to the phenomenon of compounded conservatism: The resulting estimates correspond to the upper bound of a confidence interval whose probability is far, far greater than the probabilities of each of the components used to construct it and which depends on arbitrary factors like the number of parameters included in the risk assessment.*

The conservatism embodied in the derivation of HHWQC is discussed in greater depth in Attachments H and I. As States consider changing the values used for the various parameters used to derive HHWQC (even when choosing values that, by themselves, are less stringent than those used by USEPA to derive the 2015 HHWQC), they should keep in mind the effect of compounded conservatism and whether they are meeting or exceeding the risk management goals upon which their State-specific HHWQC are based. Application of probabilistic risk assessment, see Section 8 below, can help States demonstrate that risk management goals are being met.

8 PROBABILISTIC RISK ASSESSMENT

Traditionally, HHWQC have been derived by regulatory agencies using deterministic risk assessment methods (e.g., USEPA 2000). Those methods assign a single value (from a range of possible values) to each parameter in an equation that yields an HHWQC. Parameters include those used to estimate exposure, potential toxicity, and allowable risk level. Many people view the selection of the allowable risk level as the only risk management decision in the setting of HHWQC. That is incorrect. Selecting a single value from a range entails an element of subjectivity and is often a topic of debate (Finley and Paustenbach 1994, Burmaster et al. 1995). In the context of setting criteria, selection of a single input value from a range of values represents a risk management decision or science policy choice. Unfortunately, the effect of the choice relative to the intended risk management goal is not always apparent.

Because regulatory agencies tend to err on the side of protecting public health, the derivation process typically incorporates the selection of conservative values (i.e., high-end or maximum values) for several parameters establishing the HHWQC (USEPA 1989b, 1991b, 2011), which leads to compounded conservatism (see Section 7). When using a deterministic risk assessment approach, it is impossible to discern the degree to which HHWQC are more protective than implied by the risk management goal and

the actual level of protection afforded different segments of the population. Probabilistic risk assessment (PRA) is an alternative to the traditional deterministic risk assessment methods. It uses a range of values for one or more input parameters thereby reducing the need for risk management decisions inherent to the selection of a single value for each parameter. Because the outcome of PRA is a distribution of risk, it makes the risk management decisions (i.e., the level of protection afforded different segments of the population) more transparent within the HHWQC derivation process.

The commonly used deterministic HHWQC derivation process uses equations that estimate exposure and risk associated with consumption of water and fish from surface water. Deterministic HHWQC are derived using equations that include both exposure and toxicity parameters combined with a risk management goal (i.e., an acceptable risk level for either carcinogenic or non-carcinogenic effects). Probabilistic HHWQC are derived by using these same equations, combined with distributions for one or more parameters representing the inherent variability in a population's physical characteristics and behaviors, or the uncertainty surrounding a parameter, to generate a distribution of risk. The HHWQC derived using probabilistic methods is the water concentration that has associated with it a distribution of potential risk that has better alignment with the risk management goal(s) selected by the regulatory agency. In some cases, a regulatory agency may select a single risk management goal. For example, a regulatory agency might require that the hazard quotient (HQ) for the 90^{th} percentile of the population be equal to or less than 1.0 (e.g., FDEP 2016). Alternatively, a regulatory agency may select multiple risk management goals that need to be met by an HHWQC. For example, that the arithmetic mean of the population must have an excess lifetime cancer risk (ELCR) equal to or less than $1x10^{-6}$, that the 90^{th} percentile of the population must have an ELCR equal to or less than $1x10^{-5}$, and that highly exposed populations have an ELCR no greater than $1x10^{-4}$, as did FDEP (2016).

Monte Carlo Analysis (MCA) is used to generate a distribution of risk when one or more input variables are defined as probability distributions. This technique has been widely used in engineering, finance, and insurance as an alternative to solving equations with probability distributions analytically, which is mathematically complex (USEPA 2001). MCA is easily accomplished using commercial software (e.g., @Risk or Crystal Ball). The computer randomly selects input values from each probability distribution and solves the equation to calculate risk; this process is called an iteration. Typically, a large number of iterations are performed (e.g., 10,000 or more). One set of iterations is called a simulation. After the simulation is complete, the resulting risk estimates form a distribution of potential risk that can be compared to the target risk management goal(s).

Deriving HHWQC using PRA does not mean that HHWQC will necessarily be higher (or lower) than a deterministically derived HHWQC. A key determinant of whether probabilistically derived HHWQC are higher or lower than deterministically derived HHWQC is the choice of health protection target. Using the same input distributions, two risk managers could derive two entirely different sets of probabilistically based HHWQC, varying only in the target risk level and target population percentile chosen.

USEPA (2000) indicates that "An important part of risk characterization…is to make risk assessment transparent. This means that conclusions drawn from science are identified separately from policy judgements and risk management decisions, and that the use of default values or methods, as well as the use of assumptions in risk assessments, are clearly articulated." Because PRA can employ the full the range of values for parameters that determine HHWQC and the output is the full range of potential risk, decisions about the level of protection afforded different segments of the population is transparent, and the transparency of the distinction between science and policy is better achieved than when using

deterministic approaches. When deriving HHWQC, States should consider the benefits of using PRA. Many of these benefits have been documented by USEPA (USEPA 2014b). As demonstrated by FDEP (2016), the necessary inputs for key parameters are available as are the computational tools to run probabilistic analyses. The use of PRA to derive HHWQC is discussed in further detail in Attachment J.

9 HUMAN HEALTH PROTECTION TARGETS

As noted in Section 8, the selection of acceptable risk targets has a large effect on the final value of HHWQC. Deciding what level of risk is acceptable is a multi-faceted decision and reflects many smaller choices about both how to merge scientific knowledge and public policy on health protection. These choices should consider such decisions within the broader context of other the sources of risks to our health and the many consequences of excessive conservatism in environmental standards. A more detailed discussion of various perspectives that States may wish to consider when selecting human health protection targets is presented in Attachment K.

The risk of getting cancer from a lifetime of exposure to a chemical is expressed as a probability of developing cancer above and beyond the background risk that already exists, also known as the ELCR. A $1x10^{-4}$ risk (or 1E-04) is a one in ten thousand chance of getting cancer over and above the background risk assuming a lifetime of exposure; a $1x10^{-6}$ risk (or 1E-06) is a one in one million chance. These risk levels represent the upper bound probability that an individual exposed to the chemical in the environment will develop cancer as a result of that exposure. Various statutes and associated regulations define acceptable risks differently. Standards set under the Occupational Safety and Health Act to protect workers on the job reflect an ELCR on the order of $1x10^{-3}$. The limits on the concentrations of chemicals in our drinking water at the maximum contaminant levels (MCLs) allowed reflect a range of ELCRs between$1x10^{-7}$ and $1x10^{-3}$. As a result of the different ways of thinking about acceptable risk and the factors that must be taken into account when regulating exposure to chemicals, regulators have defined goals for limiting cancer risks in different ways in various regulatory programs. Table 3 summarizes benchmark criteria.

Table 3. Benchmarks for Acceptable Risk

Law / Regulation	Focus	Risk Standard	Criterion for Carcinogens
Clean Water Act	Surface water	Adverse health impacts	$1x10^{-4}$ to $1x10^{-6}$
Safe Drinking Water Act	Public drinking water	Any adverse effect	Goal: 0
			Enforceable standard: >$1x10^{-4}$ to $1x10^{-7}$
Toxic Substances Control Act	Chemicals manufactured or imported into the United States	Unreasonable risk	$1x10^{-4}$ (inferred, absent clear policy)
Occupational Safety and Health Act	Worker protection	Significant risk over 45-year working life	$1x10^{-3}$
Comprehensive Environmental Response, Compensation, and Liability Act, or Superfund	Uncontrolled hazardous waste sites	No significant risk	$1x10^{-4}$ to $1x10^{-6}$

Regarding HHWQC, USEPA (2000) states:

> *EPA also believes that criteria based on a 10^{-5} risk level are acceptable for the general population as long as States and authorized Tribes ensure that the risk to more highly exposed subgroups (sportfishers or subsistence fishers) does not exceed the 10^{-4} level.*

Deterministic HHWQC are set at a single acceptable risk level. When using the deterministic approach, a common interpretation is that everyone is protected at the chosen acceptable risk level. However, the reality is that for any exposed population, there exists a distribution of risk, because risk varies with each person's attributes and lifestyle. With a probabilistic approach, a regulatory agency has the ability to set acceptable risk levels for one or more segments of the population, as discussed in Section 8. This leads to an increased level of transparency regarding which segments of the population are protected at which levels. Use of the probabilistic approach instead of the deterministic approach does not necessarily change the level of risk for members of the population, it just makes the various risk levels clear to the user rather than being hidden behind a single value.

USEPA, in its probabilistic risk assessment guidance for Superfund sites (USEPA 2001), suggests that risk managers target population percentiles between the 90th and 99.9th (with a preference for the 95th) at acceptable risk levels between 1x10^{-6} and 1x10^{-4}. Oregon, the only State with its own PRA guidance,

Table 4. Odds of Dying from Various Causes

Cause of Death	Odds of Dying	Lifetime Risk
Heart Disease and Cancer	1 in 7	1.4x10^{-1}
Chronic Lower Respiratory Disease	1 in 27	3.7x10^{-2}
Intentional Self-harm	1 in 97	1.0x10^{-2}
Unintentional Poisoning by and Exposure to Noxious Substances	1 in 103	9.7x10^{-3}
Motor Vehicle Crash	1 in 113	8.8x10^{-3}
Fall	1 in 133	7.5x10^{-3}
Assault by Firearm	1 in 358	2.8x10^{-3}
Pedestrian Incident	1 in 672	1.5x10^{-3}
Unintentional Drowning and Submersion	1 in 1,183	8.5x10^{-4}
Exposure to Fire, Flames or Smoke	1 in 1,454	6.9x10^{-4}
Choking from Inhalation and Ingestion of Food	1 in 3,408	2.9x10^{-4}
Pedacyclist Incident	1 in 4,337	2.3x10^{-4}
Exposure to Excessive Natural Heat	1 in 10,784	9.3x10^{-5}
Exposure to Electric Current, Radiation, Temperature and Pressure	1 in 14,695	6.8x10^{-5}
Cataclysmic Storm	1 in 63,679	1.6x10^{-5}
Contact with Hornets, Wasps and Bees	1 in 64,706	1.5x10^{-5}
Being Bitten or Struck by a Dog	1 in 114,622	8.7x10^{-6}
Lightning Strike	1 in 174,426	5.7x10^{-6}

Notes:

National Safety Council. 2016. Injury Facts: Odds of Dying. Retrieved from http://www.nsc.org/learn/safety-knowledge/Pages/injury-facts-odds-of-dying.aspx

requires that an ELCR of 1x10^{-6} be met at the 90th percentile and an ELCR of 1x10^{-5} be met at the 95th percentile (ODEQ 1998). Florida, the only State to have employed PRA to derive HHWQC, did so by targeting a 1x10^{-6} risk level for the mean of the population, 1x10^{-5} for the 90th percentile, and ensuring that the most exposed Floridians do not exceed an ELCR of 1x10^{-4}.

To develop a more concrete sense of 1x10-6 or one in one million, researchers have compiled data on various causes of death (Table 4)[8], from ones that are common to ones that are rare.

Table 5. Background Cancer Incidence Compared to Hypothetical Lifetime Cancer Incidence Associated with a Range of Target Risks

Population Background	Hypothetical Increased Lifetime Cancer Incidence			
	$1x10^{-7}$	$1x10^{-6}$	$1x10^{-5}$	$1x10^{-4}$
40%	40.00001%	40.0001%	40.001%	40.01%

Another perspective when thinking about allowable risk is to consider the change in lifetime cancer incidence associated with a particular, allowable risk level. In the United States, about 40% of the population is expected to develop some kind of cancer over the course of his or her lifetime. The comparison illustrated in Table 5 shows the lifetime increased incidence of cancer associated with various alternative allowable cancer risks. In terms of biologically measurable impacts on cancer incidence or on public health, the various allowable risk levels shown in Table 5 are indistinguishable.

10 SUMMARY

USEPA's 2015 National HHWQC revised many of the inputs used to derive the pre-2015 national HHWQC. Some of the revisions USEPA used when deriving the 2015 HHWQC were based on new science and data, others were based on science policy decisions, and others were a mix of the two. This report has presented background information on many of those inputs with a focus on new data and science. The goal of the background information is to provide State regulators a broader perspective of the data and science surrounding the inputs discussed in this report and, in the process, identify areas where the assumptions used by USEPA to develop the 2015 National HHWQC may not be applicable to the waters of specific States.

USEPA's assumptions may not be applicable for a variety of reasons. They may not be representative of a State's surface waters (e.g., State-specific DOC and POC concentrations may differ from national averages). The fish consumption rates of a State's population may differ from the national average. The BAF methodology, which is based on the bioaccumulation of PCBs in the Great Lakes and its food web, may not be representative of the waters in a State. A State's waters may not support the kinds of fish used by USEPA in the national FCR or when estimating the National BAF. Both the national FCR and the National BAF include trophic level 2 species comprised exclusively of invertebrates/shellfish such as shrimp, clams and lobster. These species are not present and consumed from inland waters.

[8] It is important to keep in mind that the comparisons presented in this section are to risk of death from other causes. The allowable risks used to derive HHWQC represent the hypothetical increased risk of getting cancer, not of dying of cancer. The latter risk would be smaller. In other words, if an HHWQC is based on an allowable risk of $1x10^{-6}$ of getting cancer, the chance of dying of cancer might be one third of that ($3x10^{-7}$), if one assumes that one third of all cancers are fatal.

Additionally, some of the procedures used by USEPA to develop the inputs used to derive the 2015 National HHWQC are not transparent and may not be appropriate. The lack of transparency is particularly evident when trying to discern the effect on the National FCR of the apportioning of species between marine and nearshore habitats. USEPA has not provided sufficient information (specifically, species-specific FCRs) for States and other interested parties to develop FCRs with different apportionment of species to include in a FCR. Examples of potentially inappropriate assumptions from the BAF methodology include; the assumption that accumulation of chemicals in invertebrates such as water fleas and mayflies is representative of accumulation in shellfish consumed by humans (e.g., shrimp); and the application of a foodchain multiplier to PAHs and other substances when those compounds are known to be metabolized by fish.

A priori, one cannot predict whether consideration of the information presented in this report, and other information States may have available to them, to establish scientifically defensible inputs will result in State-specific HHWQC that are higher or lower than USEPA's 2015 National HHWQC. Given the large number of inputs upon which HHWQC depend, the diversity of waters, food webs, and characteristics of State-populations across the United States, and the large number of chemicals involved, it is likely that some State-specific HHWQC will be higher than USEPA's 2015 National HHWQC and others will be lower. The goal of this report is to provide States with information that allows them to establish State-specific HHWQC that meet each States' human health protection targets and are based on the best science available.

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ATTACHMENT A

Report on Selected Aspects of EPA's Draft 2014 Update of Human Health Ambient Water Quality Criteria

In May 2014, USEPA released draft updated recommended HHAWQC for 94 chemical substances. This attachment contains excerpts from an Arcadis report entitled *Report on Selected Aspects of EPA's Draft 2014 Update of Human Health Ambient Water Quality Criteria*. The remaining sections of *Report on Selected Aspects of EPA's Draft 2014 Update of Human Health Ambient Water Quality Criteria* are not relevant to the methodology USEPA used to derive the 2015 National HHAWQC and are not included in this attachment.

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Report on Selected Aspects of EPA's Draft 2014 Update of Human Health Ambient Water Quality Criteria

Docket Number: EPA–HQ–OW–2014–0135

Prepared for Federal Water Quality Coalition (FWQC)

August 13, 2014

Report on Selected Aspects of EPA's Draft 2014 Update of Human Health Ambient Water Quality Criteria

Docket Number: EPA–HQ–OW–2014–0135

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Table of Contents

Comment 1. Marine species should not be included in the fish consumption rate used to develop the draft updated HHWQC.

Summary: Dilution provided by the large volume of water, tides, and ocean currents present in most near shore waters indicates that concentrations of chemicals regulated by HHWQC in near shore waters will be small compared to concentrations present in fresh and estuarine waters. Additionally, marine species caught in such waters may not have been present in such waters for a long enough time to have accumulated tissue concentrations assumed by the HHWQC. As a result, concentrations of chemicals in marine fish caught in near shore waters are likely to be much lower than assumed by the draft updated HHWQC. Regardless, the chemical-specific body burdens in true marine species reflect bioaccumulation in the marine environment, which is outside the jurisdictional control of States and authorized Tribes. This means that including any marine species in the UFCR would result in HHWQC that, almost by definition, can never be achieved based on actions any one state, or any group of states, could take. Based on these observations we recommend that EPA continue its past practice of excluding marine fish from the UFCR used to derive the draft updated HHWQC. If marine fish are to be included we recommend EPA provide data and analyses demonstrating that tissue concentrations in marine fish caught in near shore waters are larger than tissue concentrations of such fish caught in open oceans.

Discussion: The UFCR used to develop the draft updated HHWQC incorporates marine species under the pretext that fish classified as marine but caught in near shore waters represent "local" fish that could be affected by chemicals at a concentration equal to the draft updated HHWQC. The key assumption is that near shore waters (within approximately three miles of the shoreline) have concentrations of chemicals equal to the draft updated HHWQC and that the fraction of marine species harvested from such near shore waters have spent sufficient time in such waters to have their tissue concentrations be in equilibrium with the concentration in the near shore waters, where the equilibrium concentration is defined by the BAF. Neither of these assumptions is likely to be representative of near shore waters and, thus, of marine fish harvested from such waters. In fact, the chemical concentrations in such waters and marine fish caught from such waters are likely to be much lower than assumed by the draft updated HHWQC.

To the extent near shore waters are affected by concentrations of chemicals regulated by HHWQC, those chemicals are present in such waters because they were discharged in a freshwater environment, transported to the near shore waters by way of a river, and then released into the near shore waters at the mouth of the river. Even

if one assumes that the concentration of the chemical in the river water at its mouth prior to release to the ocean is equal to the HHWQC, which is a very unrealistic assumption given that most discharges are diluted by river flow, the concentration in the near shore waters will be greatly diluted by the volume of the ocean, tidal exchange, and ocean currents. Therefore, the concentration of chemicals in near shore waters as defined by EPA will be substantially lower than the HHWQC. Indeed, the concentrations may be so much lower as to not to lead to a material increase in exposure.

Moreover, concentrations of many chemicals in mussels and oysters collected from near shore waters have been decreasing over the past two decades or more (O'Conner and Lauenstein 2006). EPA should provide data justifying the need to include potential exposures associated with fish caught from near shore waters in the draft updated HHWQC when such fish were not included when the existing HHWQC were established and concentrations of chemicals in near shore biota were higher.

We recommend that EPA provide an evaluation of the potential contribution of freshwater releases to near shore waters to document the need for inclusion of marine fish. If near shore waters are shown to be affected by freshwater releases approaching the HHWQC, EPA should then document that the marine species caught in those waters have or are expected to have concentrations that are in equilibrium with the water concentrations. This will depend upon assumptions about uptake and depuration and time spent in the near shore waters versus open ocean waters. EPA needs to provide specific examples of species for which this is a concern and why those examples are likely to be representative of other (all) marine species harvested in near shore waters.

We acknowledge that ocean discharges represent a possible special, localized condition. EPA should examine how many such discharges occur and how the volume compares to freshwater discharges. EPA should also document that harvesting of marine fish occurs near such discharges. If such discharges are frequent enough and of a large enough magnitude to warrant consideration when setting HHWQC, we recommend that EPA develop a process that is transparent enough and flexible enough that regulatory agencies responsible for establishing allowable water concentrations can use the approach recommended by EPA to establish more stringent site-specific HHWQC for such situations. The special case of ocean discharges should not be the basis for including marine fish in the UFCR, assuming such discharges require such inclusion in the first place.

The above comments suggest that it is very unlikely that marine fish caught in near shore waters can be considered to have the same potential to accumulate chemicals as fish that reside in and are caught in fresh and estuarine waters. Based on the reduced potential, we recommend that EPA exclude marine fish from the UFCR, and that if marine fish are to be included, EPA provide data and analyses that demonstrate such exposures are material and need to be accounted for by HHWQC.

Comment 2. EPA has not adequately documented its methodology for estimating fish consumption rate and life-cycle apportionment for marine species.

Summary: The apportionment of species to freshwater, estuarine, and marine habitats is not thoroughly documented by EPA. We recommend that EPA make transparent the process by which the apportionment was conducted such that members of the public interested in the process can duplicate EPA's findings and determine the fraction of the overall fish consumption rate that is comprised of freshwater and estuarine fish versus marine fish. To facilitate this we recommend that EPA provide a summary of the commercial landings data, species-specific life history data, and species-specific fish consumption data EPA used to arrive at the apportionments shown in Table 1 of EPA (2014).

Discussion: In contrast to EPA's existing HHWQC that do not include marine fish when deriving HHWQC, EPA's draft updated HHWQC are based on a fish consumption rate that includes a contribution from marine fish. That contribution is based on apportioning the fraction of marine species that are harvested in estuarine and near shore waters versus open ocean waters. The habitat apportionment process is poorly documented. Furthermore, for anadromous fish (i.e., those that spend part of their lives in marine waters and part of their lives in estuarine and near shore waters), this assumption oversimplifies the process by which the chemical body burdens of fish are accumulated.

EPA (2014) states that the assignments of species to freshwater, estuarine, and marine habitats were completed by a fisheries biologist. While Appendix A of EPA (2014) provides the results of this analysis, the methodology that was used to arrive at these assignments is not clear. For select species, EPA (2014) states that it used NOAA landings data to apportion the species-specific consumption rate to various habitats. However, for a number of species, what appear to be generalized habitat apportionments are assigned without a strong scientific basis. For example, grouper are apportioned 50% estuarine and 50% marine, with the note that there are "150

species", some of which are "marine only, some estuarine and marine." Similarly, rockfish are apportioned 50% estuarine and 50% marine, with a similar note simply indicating that "approximately half are found in estuaries (in addition to marine habitats)." Scallops are assigned as entirely estuarine. However the NMFS landings data referred to by EPA (2014) indicate that about 99% of scallops are ocean scallops and not bay scallops (57,540,043 pounds of ocean scallops landed in 2010 and 376,827 pounds of bay scallops). Based on the landings data, scallops should be weighted almost entirely marine and not estuarine. Because species specific consumption rates are not provided, the effect of this misclassification on the UFCR used to derive the draft updated HHWQC cannot be determined. In these cases and others, the technical justification for habitat assignments needs to be clearly documented including references to life history information used to make judgments about habitat use.

While EPA (2014) recognizes that habitat apportionment is complicated by the fact that some species live in multiple habitat types at different life stages, the method used to apportion consumption of anadromous fish to estuarine/near shore and marine habitats is unclear. For example, an apportionment of 15% estuarine and 85% marine is assigned to both chum salmon and coho salmon, with a note simply indicating that "some populations spend many months in estuaries." In the past, EPA has designated Pacific salmon as marine species, effectively excluding them from the UFCR used to derive HHWQC (EPA 2002), as it was commonly accepted that salmon accrue most of their body mass and chemical body burden in marine waters. However, in recent years, the treatment of salmon and other anadromous species in the FCR used to derive WQC has been called into question (e.g., WDOE 2013). Not only are salmon of particular cultural significance in the Pacific Northwest, but their life histories are varied and complex. While all current research supports a conclusion that the majority (i.e., >90%) of the bioaccumulative chemical body burden in adult Pacific salmon is acquired in the marine phase of their life (Cullon et al. 2009, O'Neill and West 2009), this has not necessarily been proven for all anadromous fish. Therefore, there is some debate about the best approach to apportionment for these species. If EPA wishes to include some consumption of anadromous fish in the UFCR it needs to carefully weight apportionment based on residence time (i.e., apportionment of consumption based on relative amount of time each species spends in marine waters) vs. growth patterns (i.e., apportionment of consumption based on where and when each species accrues body mass) vs. catch location (i.e., apportionment of consumption based on where fish are caught). Whichever method is ultimately used, EPA should provide clear justification for it's selection, and the process as executed should be clearly and thoroughly documented so that reviewers can understand and reproduce the results.

EPA needs to provide all necessary information to enable stakeholders to reproduce the apportionment upon which the draft updated HHWQC are based. To that end, we recommend that EPA provide a summary of the landings data used in the habitat apportionment process. We also request that EPA provide the species specific UFCRs that were combined with the habitat apportionment estimates to determine the overall freshwater, estuarine, and near shore consumption rates.

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ATTACHMENT B

A Brief Review of Issues Relevant to the Accumulation of Persistent, Bioaccumulative, and Toxic (PBT) Chemicals by Salmon

A BRIEF REVIEW OF ISSUES RELEVANT TO THE ACCUMULATION OF PERSISTENT, BIOACCUMULATIVE, AND TOXIC (PBT) CHEMICALS BY SALMON

INTRODUCTION

In September 2011 Washington State Department of Ecology (WDOE) issued Publication No. 11-09-050, *Fish Consumption Rates Technical Support Document, A Review of Data and Information about Fish Consumption in Washington*. This technical support document (TSD) was generated to support decision making regarding how to obtain an appropriate fish consumption rate (FCR) for use in calculating water quality standards for protecting human health (HHWQS). One of the issues WDOE raised in this TSD was whether consumption of salmon should be included in whatever FCR is ultimately used in these calculations, and if it is concluded that salmon should be included in an FCR, how to do so.

The driver behind this is human exposure to toxic chemicals, specifically via consumption of fish (or aquatic tissue in general). The greatest risk to human health from consumption of fish is generally understood to result from the presence of persistent, bioaccumulative, and toxic (PBT) chemicals. Thus the primary factor in determining the appropriateness of including consumption of salmon in an FCR is where salmon actually pick up these contaminants. A brief review of what is known about this subject is presented herein.

WHERE SALMON ACCUMULATE PBT CHEMICALS

As discussed by NOAA (2005), different runs of salmon exhibit different life histories. More specifically, NOAA described stream-type and ocean-type life histories. Behavioral attributes of these two general types of salmon are summarized in Table 1.

Table 1. A Summary of the Juvenile Characteristics of Stream and Ocean Life History Types

Stream-Type Fish	Ocean-Type Fish
Species	
Coho salmon	Coho salmon
Some Chinook populations	Some Chinook populations
Steelhead	Chum
Sockeye	Pink
Attributes	
Long period of freshwater rearing (>1 yr)	Short period of freshwater rearing
Shorter ocean residence	Longer ocean residence
Short period of estuarine residence	Longer period of estuarine residence
Larger size at time of estuarine entry	Smaller size at time of estuarine entry
Mostly use deeper, main channel estuarine habitats	Mostly use shallow water estuarine habitats, especially vegetated ones

[SOURCE: NOAA 2005]

From Table 1, different species of salmon and different runs of the same species can exhibit distinctly different life histories, including how much time is spent in freshwater and where in freshwater systems this time is spent. These differences are potentially significant in that they may lead to differences in the mass (burden) of chemical contaminants (e.g., PBT chemicals)

ultimately accumulated by the salmon, and in the fraction of this ultimate burden accumulated in freshwater vs. saltwater. Although the latter may not be relevant when assessing the risk to human health resulting from eating contaminated fish in general, it is relevant when considering what fraction of this overall risk results from accumulation of contaminants in freshwater systems vs. saltwater systems.

This last point is directly relevant to the question of whether there is any utility in including consumption of salmon in an FCR that will be used to drive remedial action(s) on the geographically limited scale of a single state. If a significant fraction of the contaminant burden found in salmon is accumulated in true freshwater systems it makes sense that the consumption of salmon be included in an FCR. However, if accumulation in the open ocean dominates, inclusion of salmon in an FCR makes no sense because there is no action the state can take that will have a significant effect on the contaminant burden found in returning adult salmon.

Exclusion of salmon from an FCR does not imply that human exposure to contaminants due to consumption of salmon should not be accounted for when assessing overall risks to human health. Instead, these issues should be weighed when deciding whether salmon are accounted for when assessing the risks resulting from consumption of freshwater fish (by including consumption of salmon in an FCR) or when assessing the risks resulting from consumption of saltwater or marine fish (salmon would be backed out of the risk assessment for deriving a freshwater HHWQS via the relative source contribution or RSC). Ultimately, the issue of where the risks from consumption of salmon are counted appears to be an academic question. The more important factor (from the perspective of characterizing risk) is to ensure that consumption of salmon is not double counted by including it in both an FCR **and** as a component of the RSC.

In any case, the issue of salmon (or anadromous fish in general) is unique in that it is quite likely that a generic salmon will accumulate contaminants in both freshwater and saltwater habitats, and that the relative fraction accumulated in one habitat vs. the other will vary with species, run, and even individual. Taken to the extreme, this implies that each run needs to be evaluated independently to determine where contaminants are accumulated. However, much of the scientific literature supports accumulation in the open ocean as the dominant pathway for uptake of PBT chemicals by salmon, with the work of O'Neill, West, and Hoeman (1998), West and O'Neill (2007), and O'Neill and West (2009) providing perhaps the most through examination of the issue.

Figure 1 is taken from O'Neill and West (2009) and shows that levels of polychlorinated biphenyls (PCBs) in adult Chinook salmon (fillets) collected from a wide range of geographic locations are relatively uniform except for fish taken from Puget Sound, which show three to five times higher levels of PCBs than fish taken from other locations. As discussed by the authors, these data can be interpreted as indicating accumulation of PCBs in Puget Sound and/or along the migratory routes of these fish, which, depending on the specific runs, can pass through some highly contaminated Superfund sites (e.g., Duwamish Waterway). However, O'Neill and West (2009) concluded that, on average, >96% of the total body burden (mass) of PCBs in these Puget Sound Chinook was accumulated in the Sound and not in natal river(s).

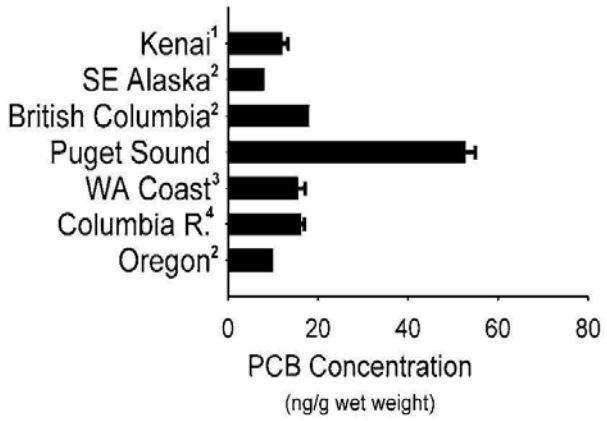

Figure 1. Average (±SE) PCB Concentration in Chinook Salmon Fillets
Data for Puget Sound were based on 204 samples collected by the Washington Department of Fish and Wildlife from 1992 to 1996; data for other locations were taken from the following (indicated by superscript numbers): [1]Rice and Moles (2006), [2]Hites et al. (2004; estimated from publication), [3]Missildine et al. (2005), and [4]United States Environmental Protection Agency (USEPA 2002)
[SOURCE: O'Neill and West 2009]

The basis for this conclusion is presented in Table 2, which compares PCB concentrations and body burdens in out migrating Chinook smolts collected from the Duwamish River and adults returning to the Duwamish.

TABLE 2.—Concentration of PCBs (ng/g) and body burden of PCBs (total ng/fish) in out-migrating Chinook salmon smolts and returning adults from the contaminated Duwamish River, Washington.

Variable	Smolts	Adults
Number of samples	80	34
Mean fish weight (g)	10	6,000
Whole body PCB concentration (ng/g)[a]		
Mean	170	57
95th percentile	860	88
PCB body burden (ng/fish)[a]		
Mean	2,100	350,000
95th percentile	9,200	800,000
Mean % of PCB body burden from the most contaminated smolts[b]	—	3.8

[a] Values for smolts are from J. P. Meador (National Oceanic and Atmospheric Administration Fisheries, Northwest Fisheries Science Center, personal communication); values for adults were estimated from measured muscle tissue concentration using the fillet–whole-body regression (see Methods) for PCBs.
[b] Contaminant data were only available for out-migrating subyearling smolts, so only samples with adults that went to sea as subyearlings were included in the analysis.

[SOURCE: O'Neill and West 2009]

These data show that even the most contaminated out migrating smolts contained no more than 4% of the body burden (mass) of PCBs found in returning adults. Thus, >96% of the PCB mass (burden) found in the returning adults was accumulated in Puget Sound. Even allowing for an order of magnitude underestimate in the body burden of out migrating smolts, O'Neill and West (2009) concluded that accumulation in freshwater would account for <10% of the average PCB burden ultimately found in adults returning to the Duwamish. By extension, this analysis supports the conclusion that Chinook salmon passing through uncontaminated estuaries during out migration accumulate a dominant fraction of their ultimate PCB body burdens in the open ocean. Other researchers have also reached this conclusion using their own data (e.g., Johnson et al. 2007; Cullon et al. 2009).

However, this analysis does not explain why Chinook salmon collected in Puget Sound exhibit higher concentrations of PCBs than Chinook salmon collected from other locations (Figure 1). Ultimately, O'Neill and West (2009) attributed this to a combination of factors, specifically PCB contamination of the Puget Sound food web (e.g., West, O'Neill, and Ylitalo 2008) combined with a high percentage of Chinook displaying resident behavior. That is, a large fraction of out migrating Chinook smolts take up permanent residence in the Sound, where they feed from a more contaminated food web than found in the open ocean. These factors would not affect Chinook runs or runs of any other species associated with natal rivers that discharge to saltwater outside Puget Sound.

Overall, these data support the position that, as a general rule, the predominant fraction of the ultimate PCB burden found in harvested adult fish is accumulated while in the ocean-phase of their life cycle (e.g., Cullon et al. 2009; Johnson et al. 2007; O'Neill and West 2009). Although this conclusion is specific to PCBs, there is no reason to suppose that it would not also hold for other legacy PBTs (e.g., DDT, dioxins) or globally ubiquitous PBTs (e.g., PBDEs, methylmercury) in general (e.g., Cullon et al. 2009). Because concerns about human consumption of fish are driven by risks from exposure to PBTs, driving the FCR higher by including salmon would thus appear to be of limited utility from the perspective of protecting human health simply because these contaminants are accumulated in the ocean.

With that said, there are sufficient data to conclude that the food web in Puget Sound is contaminated with PCBs to a greater degree than the food web in the open ocean. To the extent that this is a result of true local sources (e.g., sediment hotspots), there may in fact be some "local" action that can be taken to reduce PCBs, or potentially other PBTs, in Puget Sound salmon. However, this is totally dependent on identification of localized sources amenable to remediation, and not simply a conclusion that the food web is contaminated (e.g., West and O'Neill 2007).

Again, simply increasing the FCR by including salmon will have essentially no positive effect on human health given that the dominant fraction of PBT body burdens in salmon appears to be accumulated in the open ocean, and not in waters immediately subject to in-state loadings.

PBT ACCUMULATION BY DIFFERENT SALMON SPECIES

As discussed, there is ample evidence that the body burdens of PBTs found in returning adult Chinook salmon depend to a significant extent on the life history of the specific run. Beyond this, there are interspecies differences in migratory and feeding behavior that suggest Coho, sockeye, pink, and chum salmon will not accumulate PBTs to the same extent as Chinook

salmon under similar exposure scenarios (Groot and Margolis 1991; Higgs et al. 1995). Perhaps the most significant factor differentiating Chinook from the other salmon species is that Chinook tend to eat more fish (Higgs et al. 1995). Thus they effectively feed at a higher trophic level than the other species of salmon, and would be expected to accumulate greater burdens of PBT chemicals even when sharing the same habitat. This is in fact observable. For example, when looking at adult Chinook and Coho returning to the same rivers, O'Neill, West, and Hoeman (1998) found that Chinook muscle contained, on average, almost twice the total PCB concentrations found in Coho muscle. This was also true for adults collected in Puget Sound proper (O'Neill, West, and Hoeman 1998).

Differences between species can also manifest in sub-adults. For example, Johnson et al. (2007) reported ΣPCB concentrations in juvenile wild Coho collected from five different estuaries ranging from 5.9 to 27 ng/g (wet weight; whole body minus stomach contents). The corresponding range for wild Chinook juveniles collected from the same estuaries was 11 to 46 ng/g (wet weight; whole body minus stomach contents). Overall, PCB concentrations in juvenile Coho were, on average, equivalent to nominally 50% of those found in the paired Chinook juveniles. This is essentially the same ratio observed by O'Neill, West, and Hoeman (1998) in adult fish.

All this indicates that PBT residues in salmon will vary within species depending on the specific run, and between species regardless (i.e., even when different species share the same general habitat). Thus, grouping all salmon together does not provide an accurate assessment of PBT doses delivered to human consumers due to consumption of salmon. This suggests that human health risk assessments should, as a general rule, incorporate salmon on a species-specific basis, if not a run-specific basis.

Certainly, none of this is supportive of adopting a single default value for the dose of any contaminant received by humans via consumption of salmon. Thus adoption of a single default FCR for salmon is also not supported.

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ATTACHMENT C

Analysis of the Application of the Relative Source Contribution to Derivation of Human Health Water Quality Criteria

Analysis of the Application of the Relative Source Contribution to Derivation of Human Health Water Quality Criteria

(NCASI, July 2016)

Background

Some equations used to derive human health-based water quality criteria (HHWQC) include a parameter termed the Relative Source Contribution (RSC). The RSC describes the contribution of a contaminant from one or more sources relative to a total exposure from all sources. The Agency's justification for including RSCs in criteria for drinking water and HHWQC is provided in several documents. Related statements from some of these are as follows:

> "To determine the RMCL [Recommended Maximum Contaminant Level], the contribution from other sources of exposure, including air and food, should be taken into account." (EPA 1985)
>
> "The 1980 AWQC National Guidelines recommended that contributions from non-water sources, namely air and non-fish dietary intake, be subtracted from the Acceptable Daily Intake (ADI), thus reducing the amount of the ADI 'available' for water-related sources of intake." (EPA 2000).
>
> "EPA emphasizes that the purpose of the RSC is to ensure that the level of a chemical allowed by a criterion or multiple criteria, when combined with other identified sources of exposure common to the population of concern, will not result in exposures that exceed the RfD or the POD/UF". (EPA 2000).
>
> ". . . to ensure that the level of a contaminant in drinking water, when combined with other sources of exposure (e.g. food and air) will not result in a total exposure for an individual that exceeds the reference dose." (GAO 2011).

Consistent with the above statements, the RSC is a factor multiplied by the reference dose (RfD) for the purpose of apportioning only part the RfD to, in the case of HHWQC, exposure through consumption of drinking water and fish. This parameter has been discussed as part of HHWQC derivation since 2000 (EPA 2000), though between 2000 and 2015 a value of 1.0 (i.e., 100% and effectively negating the RSC) was most commonly used when calculating EPA's recommended HHWQC criteria (EPA 2002). Only recently did EPA incorporate the RSC for most of the relevant criteria (EPA 2015a) and also apply upper and lower-bound limits on the RSC, 80% and 20%, respectively.

For purposes of deriving HHWQC, EPA has established two procedures for calculating the RSC, the "subtraction" method and the "percentage" method. In the subtraction method, the exposure supported by the RfD is allocated among various sources by first subtracting all exposure routes other than drinking water and fish consumption and then allocating the remainder of the RfD to drinking water and fish consumption. The percentage method is a simple ratio of exposure via

drinking water and fish consumption to the total exposure. EPA has developed a decision tree for choosing both the method and ultimate value of the RSC (Table 4.1 in EPA 2000). In most cases, EPA recommends the use of the percentage method. EPA's policy preference for the percentage method is evident (EPA 2000, GAO 2011, EPA 2015b), though the justification, particularly as it relates to the existence of other media criteria, is unclear.

The purpose of this paper is to contrast these methods mathematically and in context with the purpose for establishing an RSC.

The Subtraction Method

EPA's 2000 HHWQC guidance (EPA 2000) does not contain an equation for calculating the RSC using the subtraction method. Rather it is described as: "In the subtraction method, other sources of exposure (i.e., those other than the drinking water and fish exposures) are subtracted from the RfD (or POD/UF)." Thus, it would appear that the intent of this method is to apportion the remainder of the RfD (i.e., the RfD-supported exposure less other, non-drinking water and fish exposures) to drinking water and fish exposures. Examples of the calculation methodology are provided in two, more recent documents (GAO 2011, USEPA 2015b).

The example described in GAO 2011 (for drinking water) is:

1. subtract all non-drinking-water exposures from the reference dose to determine the amount of the reference dose "available" for exposure through drinking water,
2. determine what percentage of the reference dose that remainder represents, and
3. apply the resulting percentage as the relative source contribution.

The example described in EPA 2015b is:

1. Calculate the RfD-supported exposure for the population of interest,
2. Subtract the exposures for drinking water + fish/shellfish
3. Determine the percentage of the RfD-supported exposure represented by the remainder
4. Apply the upper/lower bound limitation, if necessary.

Based on the descriptions of the subtraction method in both EPA (2000) and GAO 2011, the example provided in EPA 2015b appears to have been calculated incorrectly. Specifically, step 2 should show the subtraction of exposures from non-drinking water, non-fish/shellfish sources instead of the subtraction of exposures from drinking water+fish/shellfish.

Example calculations using the method described in GAO 2011 (applied to a HHWQC derivation) and the incorrect equations shown on slide No. 9 of EPA 2015b are provided in Table 1. The calculation procedure described in GAO 2011 is consistent with the stated intent of the subtraction method.

Table 1. Example of RSC Values Calculated by the Subtraction Method

Exposures	**ug/day**
RfD-supported	200
drinking water	20
fish/shellfish	30
all other foods	80
air (inhalation)	0
RSC	**%**
Method GAO 2011	(200-80)/200 = 60%
Method EPA 2015	(200-20-30)/200 = 75%

The Percentage Method

EPA's 2000 HHWQC guidance (EPA 2000) does not contain an equation for calculating the RSC using the percentage method. Rather it is described as: "the percentage of total exposure typically accounted for by the exposure source for which the criterion is being determined, . . . applied to the RfD to determine the maximum amount of the RfD 'apportioned' to that source."

Both GAO 2011 and EPA 2015b contain descriptions of the calculation procedure. These are summarized below:

The example described in GAO 2011 (for drinking water) is:

1. calculate the relative proportion of exposure from water as a percent of the total observed exposure and then
2. apply that percentage as the relative source contribution

The example described in EPA 2015b is:

1. sum the exposure from drinking water and fish/shellfish, and then
2. divide by the total of all know exposures

The two descriptions of the percentage method appear to be the same, that is: (drinking water+fish/shellfish exposure)/(total exposure). Using this equation, the data in Table 1 would yield a RSC value of (20+30)/(20+30+80) = 38%.

There are two noteworthy observations about the percentage method. First is that the equation does not include, and thus is unrelated to, the RfD. Second is that as the proportion of exposure due to drinking water+fish/shellfish decreases relative to the total exposure, the RSC gets smaller. The latter outcome appears counterintuitive relative to the justification for using RSC values in deriving HHWQC.

Discussion

EPA descriptions of the subtraction method, and at least one example of its application, indicate that the intent of the method is to ensure that the RfD is not exceeded. This is accomplished by allocating only the residual part of the exposure after non-drinking water+fish/shellfish exposures are removed. The subtraction method would allocate the entire RfD via this procedure absent EPA's existing policy to cap the RSC at 80%. Intrinsic to the subtraction method, is that as the relative exposure from other (i.e., non-drinking water+fish/shellfish) sources increases, the RSC value decreases in a manner such that the RfD value is never exceeded.

In contrast to the subtraction method, the percentage method is not linked to the RfD. This creates two important distinctions between RSCs calculated using the two methods. These are illustrated in the examples shown in Table 2. One of these relates to situations where the total exposures are well below the RfD-supported exposure and the drinking water+fish/shellfish contribution is small relative to other exposures (first grey highlighted row). In this case the percentage method calculates a very small RSC when this would seem not to be justified in the context of ensuring that the RfD is not exceeded. The implication appears to be one of ensuring that low exposures remain low irrespective of health risk.

Table 2. Examples of RSC Values Calculated by the Percentage and Subtraction Methods

RfD-supported Exposure	Water + Fish Exposure	Other Exposures	RSC, Percent method	RSC Subtrctn. Method	Total exposure before RSC	Allowed exposure after RSC (% method)[a]	Allowed exposure after RSC (Subtrctn. Method)a
100	5	90	0.05	0.10	95	95	100
100	5	50	0.09	0.50	55	59	100
100	50	5	0.91	0.95	55	96	100
100	90	5	0.95	0.95	95	100	100
100	90	50	0.64	0.50	140	114	100
100	50	90	0.36	0.10	140	126	100

[a] calculated as RfD*RSC+Other Exposures

The other distinction between the two methods is that the subtraction method always provides that the RfD is never exceeded, while the percentage method does not (see the lower two gray rows in Table 2). In situations where exposures from drinking water+fish/shellfish are a significant proportion of the RfD-supported exposure and exposure from other sources is also significant, the percentage method allows the total exposure after the application of the RSC to exceed the RfD-supported exposure. As such, the disconnect between the percentage method and the RfD can lead to exposures greater than the RfD.

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ATTACHMENT D

Relative Source Contribution (RSC) Derivation for Non-carcinogenic Parameters Evaluated for Chapter 62-302, FAC Human Health Criteria Revision

In February 2014, FDEP released a draft technical support document (TSD) for its proposed HHAWQC. This attachment contains a draft appendix developed in support of that TSD entitled *Appendix D. Relative Source Contribution (RSC) Derivation for Non-carcinogenic Parameters Evaluated for Chapter 62-302, FAC Human Health Criteria Revision.*

(DRAFT) Appendix D. Relative Source Contribution (RSC) Derivation for Non-carcinogenic Parameters Evaluated for Chapter 62-302, FAC Human Health Criteria Revision

Table of Contents

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(DRAFT)Relative Source Contribution (RSC) Derivation for Non-carcinogenic Parameters Evaluated for Chapter 62-302, FAC Human Health Criteria Revision

Purpose

The Relative Source Contribution (RSC) is a numeric value important to the derivation of human health ambient water quality criteria. Calculation of the RSC allows for a percentage of the non-carcinogen reference dose (RfD) exposure to be attributed to ambient water and freshwater and estuarine fish consumption. Through this calculation, the RSC can also account for exposures from sources other than water and freshwater/estuarine fish and shellfish ingestion such as inhalation of airborne sources or consumption of food/treated drinking water. The RSC is intended to ensure that total exposure for individuals does not exceed the RfD. The Florida Department of Environmental Protection has chosen to develop protective RSC values for non-carcinogenic compounds lacking a specific recommended RSC value generated by the United States Environmental Protection Agency. However, RSC values were not developed for endosulfan, endosulfan sulfate, endrin, or lindane because criteria to protect aquatic life uses are significantly more stringent than the human health-based criteria. Parameter-specific RSC values between 0.2 and 1.0 were developed where FDEP determined that there were adequate data to describe the exposure sources and pathways.

Methods

The USEPA's *Exposure Decision Tree for Defining Proposed RfD Apportionment* (Fig. 4-1, USEPA, 2000B) was used as the basis for the development of protective RSCs for non-carcinogenic compounds. To calculate an RSC, exposure information was assembled from literature sources to characterize the various potential exposure routes, including surface water sources (ambient sources e.g. surface water and fish) and non-surface water sources.

Parameter-specific relative source contribution (RSC) values between 0.2 and 1.0 were developed where FDEP determined that there were adequate data to describe the exposure sources and pathways. In some cases the RSC values exceed the 0.8 ceiling recommended in the EPA Decision Tree guidance. However, FDEP believes that RSC values up to 1.0 are appropriate in cases where the robustness of the data and weight of evidence support higher values. There is considerable conservatism built into the estimates and RSC values above 0.8 are fully protective of the majority of the general population.

<u>Literature Search Process Outline for Relative Source Contribution Derivation</u>

The first step in the literary review process was to identify major entities that a) are responsible for or play a role in the protection of public health in relation to exposure science and risk assessment and b) would have reliable peer-reviewed data pertaining to population exposures to the chemicals that were the focus of this analysis. The primary entities targeted for literature/information searches were:

- The Agency for Toxic Substances and Disease Registry (ATSDR)

- The World Health Organization (WHO)
- The Centers for Disease Control and Prevention (CDC)
- The United States Environmental Protection Agency (USEPA)
- The United States Environmental Protection Agency's Toxic Release Inventory Explorer Tool
- The United States National Library of Medicine's Hazardous Substances Data Bank (HSDB)
- The International Programme on Chemical Safety (IPCS)
- The United States Geological Survey (USGS)
- The United States Food and Drug Administration (USFDA)
- The California Office of Environmental Health Hazard Assessment (OEHHA)
- Peer reviewed literature sources
- FDEP technical reports and technical support documents

To begin the analysis, the toxicological profile created by the ATSDR was reviewed for each chemical/compound for which this type of documentation was available. This source was chosen to begin the analysis because it provided a comprehensive overview of information such as chemical/physical characteristics, exposure routes, health effects by exposure route, average concentrations of chemicals received through each exposure route and levels monitored in the environment, how the chemicals/compounds are released into the environment and the ultimate fate associated with that release, and how exposures differ between the general population and occupational exposures.

To fill in informational and data gaps that existed, online resources and documents provided by the Centers for Disease Control and Prevention (CDC), the United States Environmental Protection Agency (USEPA), the World Health Organization (WHO), the International Programme on Chemical Safety (IPCS), the United States Geological Survey (USGS), the United States Food and Drug Administration (USFDA), the California Office of Environmental Health Hazard Assessment (OEHHA), FDEP technical reports/technical support documents, and the United States National Library of Medicine's Hazardous Substances Data Bank (HSDB) were reviewed.

The types of documents reviewed for each major source include:

- Centers for Disease Control and Prevention: National Reports of Human Exposure to Environmental Chemicals
- The Agency for Toxic Substances and Disease Registry (ATSDR) toxicological profiles were used as the primary and initial literature resource. The documents were downloaded from the ATSDR website (http://www.atsdr.cdc.gov/toxprofiles/index.asp). Toxicological profiles are prepared in accordance with guidelines developed by the ATSDR and the EPA. The ATSDR toxicological profiles are intended to succinctly characterize the toxicological and adverse health effects information for the hazardous substance being described. Each profile identifies and reviews the key peer reviewed literature that describes a substance's toxicological properties.
- United States Environmental Protection Agency: Technical fact sheets, Ambient Water Quality Criteria Documents, National Air Toxics Assessment data, Contaminant Occurrence documents,

IRIS, Exposure Factors Handbooks (1997 and 2011) for exposure/intake rates and body weight, and other chemical-specific documents and studies.

- The United States Environmental Protection Agency's Toxic Release Inventory Tool was utilized to obtain data associated with on-site disposal and release of the chemicals included in our RSC derivation analysis. This source was chosen due to the fact that these data represent the most current and complete account of chemical disposal and release monitored by the EPA that is available, even though it is acknowledged as a non-exhaustive list of releases/disposals due to the fact that reporting requirements for facilities are not all-inclusive
- The World health Organization (WHO): Chemical-specific background documents for the development of WHO guidelines for drinking water quality. These WHO documents were reviewed after the ATSDR documents to support the information summarized by the ATSDR or to identify more recent data/information. The WHO documents were used to start the analysis, in cases where the ATSDR had not developed a toxicological profile.
- The International Programme on Chemical Safety (IPCS): Chemical-specific Concise International Chemical Assessment Documents, chemical-specific Environmental Health Criteria, and chemical-specific Health and Safety Guides
- The United States Geological Survey (USGS): Chemical-specific water-based studies
- The United States Food and Drug Administration: Total Diet Study Market Baskets 1991-3 through 2003-4, 21 CFR 175.105 U.S. SubChapter B-Food for Human Consumption; Part 175-Indirect Food Additives
- The California Office of Environmental Health Hazard Assessment: Public Health Goals for Chemicals in Drinking Water (chemical-specific documents)
- FDEP technical reports/technical support documents: Final Technical Report: Development of Cleanup Target Levels (CTLs) for Chapter 62-777, F.A.C., March 2013 Technical Support Document: Derivation of Human Health-Based Criteria and Risk Assessment; In a number of instances the soil residential direct exposure target clean-up levels developed for Chapter 62-777, F.A.C. (Contaminant Cleanup Target Levels) were utilized to represent exposure received through the soil ingestion pathway. These values were utilized under the assumption that they represent a level above which the state would initiate clean-up protocols and are characterized as a high-end exposure estimates instead of central tendencies, thus denoting conservatism.
- The United States National Library of Medicine's Hazardous Substances Data Bank: Provides a variety of chemical-specific information such as human health effects, environmental fate and exposure, chemical/physical properties etc.

Data and information relevant to human exposures, particularly in the United States and Florida, were extracted from these resources as the primary or initial literature resources. The reference and citation lists from these resources were also analyzed, particularly from a number of the major source documents (*i.e*. Toxicological Profiles, IPCS documents, HSDB overviews). These references were then queried in the State Library of Florida's electronic database and requested for retrieval. The references were thoroughly reviewed to help substantiate information and data that were

chosen to be included in the RSC derivation document; that is, these references were reviewed to ensure that the summaries provided in the major source documents were accurately characterized and interpreted by FDEP. Additionally, pertinent and often more recent peer reviewed literature that referenced these sources were also queried and reviewed to determine whether new or revised information had become available since the publication of the major source documents.

Additional queries were conducted to find quality literature to further support the estimated average daily exposure dose calculated for each exposure route, which is subsequently utilized to calculate the chemical-specific RSCs. A defined key word list was not used during this state library of Florida literature review as this was an interactive process where searches would often build upon themes previously queried. Searches primarily included mention of the chemical/compound under analysis and the exposure route of focus (*e.g.*, diet, fish, seafood, drinking water, air, atmospheric) and/or author's names/titles of articles referenced in other sources. Literature either citing or cited by key resources was also reviewed for relevance.

Information/data was then compiled individually for each exposure route. To determine the exposure-based concentration that would be used a number of elements were taken into account such as the source date associated with the exposure concentration, sample size, regionality, the level of conservatism of the exposure estimate, and the overall availability of data concerning chemical concentrations associated with exposure routes. A concerted effort was made to utilize the most current applicable data available, taking into account whether sample size was sufficient, exposure concentrations were measured in the United States or Florida, and the most conservative estimate of exposure was utilized to ensure that the public's health is fully protected.

In a few cases, exposure data, particularly dietary, from outside the United States (Europe) were used if sufficient data were lacking for the United States. In the cases when foreign population data were used, it was apparent that either the foreign population had similar exposure patterns as in the U.S. or were highly likely to be conservative (*i.e.*, overestimate exposure). When data adequacy was a concern and/or a major exposure route could not be quantified, the EPA's default RSC values of 0.8 or 0.2 were applied depending on the information available for that chemical/compound. In a few cases, a 10 fold factor was applied to a particular exposure route (*e.g.*, dietary) to take into account uncertainty or variability.

The major non-surface water sources (non-ambient sources) include dietary uptake (including marine fish), inhalation, soil, and drinking water. Dermal absorption was generally not characterized because FDEP's methodology for calculating human health criteria already accounts for dermal exposures. All exposure estimates were either taken from literature or calculated using chemical-specific concentrations in environmental media combined with standard exposure assumptions (*e.g.*, body weight, daily food intake) from USEPA Exposure Factors Handbooks (2011 or 1997). Calculated average daily doses (ADD_m) through each of the media were calculated as

$$\boldsymbol{ADD_m = C_m \times DE_m \times AF_m / BW}$$

where,

C_m = concentration for the media (*e.g.*, air, food, water, soil);
DE_m = Daily exposure (ingestion or inhalation) of the media;
AF_m = Absorption factor of the parameter via the media, if available; and,
***BW* =** Average body weight (70 kg). Body weight was not included if the DE_m is expressed in terms of mg/kg-day.

Unless otherwise noted for a given parameter the most recent exposure factors (USEPA, 2011A) were used in the calculations for RSC determination (**Table 1**).

Table 1. Exposure assumptions used to calculate relative source contribution values for individual non-carcinogenic human health parameters. Selected values are per capita means for the U.S. population.

Variable	Exposure Assumption	Value	Units	Source
BW	Body Weight	70	Kg	Chapter 7, USEPA (1997)
DE_m	Drinking Water	2.0	L/day	NRC (1977)
DE_m	Daily Breathing rate	16	m^3/day	Table 6-1, USEPA (2011A)
DE_m	Indoor Breathing rate	12.878	m^3/day	Calculated[1]
DE_m	Outdoor Breathing rate	3.122	m^3/day	Calculated[2]
DE_m	Soil Ingestion	20	mg/day	Chapter 4, USEPA (2011A)
DE_m	Dust Ingestion	30	mg/day	Chapter 4, USEPA (2011A)
DE_m	Soil and Dust combined	50	mg/day	Chapter 4, USEPA (2011A)
DE_m	Total Food Intake	29	g/kg-day[3]	Table 14-1, , USEPA (2011A)
DE_m	Fruit	1.6	g/kg-day	Table 19-3, USEPA (2011A)
DE_m	Vegetable	2.9	g/kg-day	Table 19-3, USEPA (2011A)
DE_m	Meat	2	g/kg-day	Table 11-3, USEPA (2011A)
DE_m	Dairy	6.6	g/kg-day	Table 11-3, USEPA (2011A)
DE_m	Grain	2.6	g/kg-day	Table 12-3, USEPA (2011A)
DE_m	Fish	0.22	g/kg-day	Table 11-1, USEPA (2011A)
DE_m	Fats	1.2	g/kg-day	Table 11-31, USEPA (2011A)

1. Calculated based on the faction of time indoors (0.8) multiplied by daily inhalation (16 m^3/day). The multiplier of 80% was generated from Table 16-22 (USEPA, 2011A) and was based on an average time spent indoors of 1159 minutes out of a 1440 minute day.
2. Calculated based on the faction of time outdoors (0.2) multiplied by daily inhalation (16 m^3/day). The multiplier of 20% was generated from Table 16-22 (USEPA, 2011A) and was based on an average time spent outdoors of 281 minutes out of a 1440 minute day.
3. Food-based intakes in the table above are represented in units of grams per kilogram bodyweight per day

The average daily doses for all non-surface water sources or media were summed (ADD_{total}) and compared to the parameter specific RfD. An RSC was calculated as

$$RSC = 1 - (ADD_{total}/RfD).$$

The calculated RSC was used, for purposes of human health criteria development, if exposure information for all non-surface water sources was available. In some cases, exposure routes could not be quantified, but available information on the compound strongly indicated that contamination via these routes was highly unlikely and that exposures could be safely and conservatively considered negligible. In these cases, the RSC was calculated based on the other, quantifiable exposure routes.

Beryllium

Background

Beryllium (CASRN 7440-41-7) is a naturally occurring metallic element found in environmental media such as rocks, soil, and coal (ATSDR, 2002). Mineral rocks are mined for beryllium, which is a component of many commercial products in its pure metallic form. It is also used in many alloys and as a constituent of certain compounds. Beryllium is an important element of the manufacturing process and production of military, aerospace, electronic, medical and nuclear-based commodities (Taylor *et al.,* 2003). Exposure to beryllium can occur through oral routes (food and water-based consumption), inhalation (through breathing ambient air or through incidental inhalation of beryllium-laden dust particles) and minimally through dermal exposures. The primary exposure route for the general population is oral ingestion through food-based consumption and drinking water intake; however, the most important pathway from an occupational exposure prospective is through inhalation (IPCS, 2001A). It is through this route that the U.S. Environmental Protection Agency has denoted beryllium as a group 2B probable human carcinogen (USEPA, 2013C).

Beryllium frequently forms covalently bonded compounds, many of which lack solubility in neutral environments and possess low mobility in sediments due to high sediment-water distribution coefficients (k_d) (ATSDR, 2002). According to Taylor *et al.* (2003), beryllium can be used as a pure metal, mixed with other metals to form high strength alloys, processed to form salts that dissolve in water, or processed to form oxides and ceramic materials. Beryllium can enter the environment through natural and anthropogenic sources. This element and associated beryllium-based compounds can be introduced to waterways through natural erosion and weathering of beryllium-containing rocks and through anthropogenic industrial wastewater discharges (USEPA, 2013A). Beryllium enters the atmosphere primarily through coal-burning power plants and fossil fuel combustion. According to Koolanz (2001), a study conducted by the U.S. EPA estimated 97% of beryllium released to the atmosphere is generated through these sources.

Exposure Source Determinations

Manufacturing and release

According to the U.S. EPA's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[1] of beryllium in 2011 accounted for 498.85 pounds with the majority of release/disposal occurring through fugitive air emissions and "other surface impoundments" (TRI2011, 2013A). Total reported off-site disposal or other releases[2] in 2011 accounted for 1,036.53 pounds of beryllium, with the majority of disposal/release occurring through solidification/stabilization and "other land disposal" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for beryllium in 2011 was 1,535.38 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 253.318 pounds of beryllium with the majority of disposal/release occurring through fugitive and point source air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 1,299.70 pounds of beryllium with the majority of disposal/release occurring through solidification/stabilization (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for beryllium in 2012 was 1,553.02 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

The United States Environmental Protection Agency has noted that environmental release of beryllium waste is a significant issue requiring proper assessment and documentation to control further hazard. According to the ATSDR (2002), beryllium has been found in at least 535 of the 1,613 current or former National Priority List (NPL) sites, which are denoted as the most severely contaminated hazardous waste sites across the United States.

Non-ambient Exposure Sources

Treated drinking water

Exposure to beryllium through drinking water is minimal. The United States Environmental Protection Agency has set the Maximum Contaminant Level (MCL) for beryllium in drinking water at 0.004 mg/L (USEPA, 2013A). According to the ATSDR (2002), a study conducted by the U.S. EPA showed that drinking water samples collected across the United States generally contained less than 2 trillionths of a gram for every liter of water with an average concentration of 0.19 µg/L. In

[1] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[2] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

addition, the ATSDR (2002) reported that the average concentration of beryllium in the United States for bottled water and tap water were < 0.1 µg/L and 0.013 µg/L, respectively. The tap water value of 0.013 µg/L was used for RSC calculation because it represents the most likely exposure value/ dose of beryllium in treated drinking water received by the general public. A standard water ingestion rate of 2.0 L/day and a standard body weight of 70 kg were also utilized in this calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of beryllium received through treated drinking water was 3.71 $x10^{-7}$ mg/kg-day.

Air

Although occupational inhalation of beryllium represents a higher risk to individuals due to the potential for exposure to higher beryllium concentrations at the workplace, the inhalation pathway for the general public breathing ambient air represents a more minimal risk. The United States Environmental Protection Agency's Integrated Risk Information System (IRIS) reported a reference concentration (RfC) for beryllium of 2 $x10^{-2}$ µg/m^3 (USEPA, 2013C). According to the World Health Organization (2009), ambient beryllium concentrations in rural areas range from 0.03-0.06 ng/m^3, from 0.04-0.07 ng/m^3 in suburban areas, and 0.1-0.2 ng/m^3 in urban areas. The ATSDR (2002) reported an average air-based beryllium concentration of 0.03 ng/m^3 and an average urban beryllium air-based concentration of 0.2 ng/m^3. According to U.S. EPA's 2005 National Air Toxics Assessment data, the total ambient beryllium concentration for the state of Florida was 2.65 $x10^{-5}$ µg/ m^3(USEPA, 2005A). To calculate the RSC, the beryllium-based air concentration of 0.2 ng/m^3 was utilized because it represents the most conservative estimate. A standard inhalation rate of 16 m^3/day and a standard body weight of 70 kg were also utilized in this calculation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of beryllium received through inhalation of ambient air was 4.57 $x10^{-8}$ mg/kg-day.

Soil

Beryllium is found naturally in the earth's crust, soils, rocks, and minerals. According to the ATSDR (2002), the mean concentration of beryllium in soils in the United States is 0.6 mg/kg. Florida-specific soils were reported to contain slightly lower beryllium concentrations, with values ranging from 0.01-5.92 mg/kg and an average concentration of 0.46 mg/kg (ATSDR, 2002). However, for the purposes of RSC calculation, the average concentration of 0.6 mg/kg was utilized to calculate the dose received through soil ingestion because it represents the most conservative mean estimate. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized in this calculation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of beryllium received through soil ingestion was 4.29 $x10^{-7}$ mg/kg-day.

Diet (other than fresh or estuarine fish)

Literature reviewing the beryllium concentrations in various foodstuffs is highly variable. According to Vaessen and Szteke (2000), the most likely route of introduction of beryllium into the food chain is via root, tuber, and forage crops grown in acidic soil. A value of 22.5 µg/kg wet weight was utilized in the calculation of the RSC. This value represents the median beryllium concentration

of 38 different food types compiled by Vaessen and Szteke and is a conservative estimate of dietary beryllium exposure (ATSDR, 2002; Vaessen and Szteke, 2000). This conservatism is evident through the fact that the U.S. EPA's *Health Assessment Document for Beryllium* reports that dietary exposure to beryllium is estimated to be less than 1 µg/day for the general public because beryllium is only slightly available for absorption in the gut (USEPA, 1987). A standard food intake rate of 29 g/kg-day was also utilized in this calculation (USEPA, 2011A). The resultant estimated average daily dose of beryllium received through dietary intake was 0.000653 mg/kg-day.

Exposures for potentially highly exposed populations

Certain individuals may be at risk for receiving higher levels of exposure to beryllium than the general population. Occupational exposure represents a major pathway through which individuals are in contact with higher beryllium concentrations and the inhalation exposure pathway represents the most significant route of occupational beryllium exposure. However, the dermal route also has the capacity to play a role in beryllium exposure, especially if the dermally exposed area contains an open wound or injury. Deubner *et al.* (2001), reported that dermal beryllium loading of approximately 0.000043 mg/cm^2 for beryllium machine workers can occur on a daily basis. Dermal and inhalation exposures can contribute to beryllium sensitization which can subsequently generate chronic beryllium disease. According to a study by the CDC's National Institute for Occupational Safety and Health (NIOSH) (2012), workers who have been exposed to beryllium and smoke cigarettes are potentially increasing their probability of developing lung cancer over their lifetime. Proximity to industrial sites that release beryllium wastes may also put individuals at higher risk of exposure.

Ambient Exposure Sources

According to the ATSDR (2002), beryllium does not readily bioaccumulate in aquatic biota or biomagnify through successively higher trophic chains in neutral environments. The IPCS (2001A) reported, an estimated geometric mean concentration of total beryllium in U.S. surface waters of 70 ng/L. Through a collaborative partnership between the USGS and the United States Environmental Protection Agency, national water quality assessment data from 1992-2001 were analyzed for their beryllium content. For ambient surface waters, a total of 2,379 samples were taken from 394 sites of which 0.5% of samples detected beryllium representing 2.8% of the sites under analysis (USEPA, 2009C). A median beryllium concentration of 0.0445 µg/L and a 99th percentile beryllium concentration of 11 µg/L were produced from the ambient surface water samples under analysis (USEPA, 2009C).

RSC Calculation

The estimated doses received through average daily exposure to beryllium were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 1** below.

Table 1. Estimated average daily beryllium exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg-day)
Inhalation of air	4.57×10^{-8}
Soil ingestion	4.29×10^{-7}
Treated drinking water ingestion	3.71×10^{-7}
Diet	0.000653
Estimated total daily dose	6.54×10^{-4}

The reference dose for beryllium is 2×10^{-3}mg/kg-day (USEPA, 2013C) and the estimated total non-ambient exposure of 6.54×10^{-4} mg/kg-day represents 32.7% of the RfD. The remaining 67.3% is available for allocation to surface water exposures through routes such as estuarine fish consumption. Thus, a chemical-specific RSC of 0.67 is suggested to be protective of human health and representative of beryllium exposures received through ambient sources.

Chloroform

Background

Chloroform (CASRN 67-66-3) is a colorless liquid with a pleasant, non-irritating odor and a slightly sweet taste. The majority of chloroform found in the environment comes from industry. Chloroform was one of the first inhaled anesthetics to be used during surgery, but is no longer used for that purpose today. Nearly all of the chloroform manufactured in the United States today is used in the synthesis of other chemicals. The primary application for chloroform is the production of HCFC-22 (R-22), which is used as a refrigerant and an intermediate in the production of the Teflon fluoropolymer (PTFE) (Glauser *et al.*, 2011). In 2011, an estimated 96% of the global consumption of chloroform was used in the manufacture of hydrochlorofluorocarbons. The remaining 4% of chloroform produced globally is used in the synthesis of pharmaceuticals, agricultural products, and as laboratory reagents. The potential for environmental release of chloroform is low since it is utilized as a chemical intermediate in closed systems.

Potential exposure to chloroform can occur through drinking water intake, food-based consumption, inhaling contaminated air, and through dermal contact with water (e.g., while showering, bathing, cleaning, washing, swimming). Incidental dermal contact during recreational activities is considered minor. The USEPA (2003A) evaluated general population exposure to Chloroform and provides a basis for a protective RSC.

Exposure Source Determinations

Manufacturing and release

Chloroform is found in waste water from sewage treatment plants, drinking water, and paper mills to which chlorine has been added. Chlorine is added to most drinking water and many waste waters to kill bacteria. Small amounts of chloroform are formed as an unwanted by-product during the process of adding chlorine to water. Chloroform can enter the air directly from factories that produce or utilize it in manufacturing processes and via evaporation from contaminated water and soils. Chloroform can enter water and soil when waste water that contains chlorine is released into these types of environmental media. Chloroform may also enter water and soil from spills and waste site/storage tank leakage.

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[3] of chloroform in 2011 accounted for 416,704.14 pounds with the majority of release/disposal occurring through point source air emissions, fugitive air emissions, and underground injection into Class I wells (TRI2011, 2013A). Total reported off-site disposal or other releases[4] in 2011 accounted for 39,799.41 pounds of chloroform with the majority of disposal/release occurring through unknown methods (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for chloroform in 2011 was 456,503.54 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 407,943 pounds of chloroform with the majority of disposal/release occurring through point source emissions, fugitive air emissions, and underground injection into Class I wells (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 25,102.25 pounds of chloroform with the majority of disposal/release occurring through unknown methods (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for chloroform in 2012 was 433,045.25 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

[3] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[4] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

Non-ambient sources of chloroform exposure considered as important and quantified by the USEPA (2003A) include treated drinking water, indoor inhalation exposure, inhalation while showering, dermal exposure while showering, inhalation of outdoor air, and dietary exposures. Chloroform concentrations for the various media were taken from USEPA (2003A).

Treated drinking water

The United States Environmental Protection Agency has estimated that a mean chloroform concentration of 24 µg/L exists in treated drinking water (USEPA, 2001). For the purposes of RSC calculation, this concentration was utilized to estimate an average daily exposure dose. A standard drinking water intake rate of 2.0L/day and a standard body weight of 70 kg were also utilized in this calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of chloroform received through drinking water intake was 6.86 x 10^{-4} mg/kg-day.

Air

Revised indoor and outdoor inhalation rates were calculated using information from USEPA (2011A). Average time spent indoors and outdoors of 19.32 and 4.68 hours/day, respectively and average breathing rate of 16 m^3/day were used by FDEP to recalculate a total daily exposure for chloroform.

General indoor air exposure to chloroform was estimated at 0.35 µg/kg-day (3.5 x 10^{-4} mg/kg-day). The assumptions utilized to calculate this exposure dose were a mean indoor air chloroform concentration of 3.0 µg/m^3, an indoor breathing rate of 12.88 m^3/day, a 0.63 inhalation fraction, and standard body weight of 70 kg (USEPA, 2003A; USEPA, 2011A; USEPA, 1997).

Outdoor air exposure to chloroform was estimated at 0.04 µg/kg-day (4.0 x 10^{-5} mg/kg-day). The assumptions utilized to calculate this exposure dose were a mean outdoor concentration of 1.6 µg/m^3, an outdoor breathing rate of 3.12 m^3/day, a 0.63 inhalation fraction, and a standard body weight of 70 kg (USEPA, 2003A; USEPA, 2011A; USEPA, 1997).

Inhalation and dermal exposure through showering

Inhalation and dermal exposures while showering of 0.14 and 0.12 µg/kg-day (1.4 x 10^{-4} and 1.2 x 10^{-4} mg/kg-day), respectively, were calculated by the USEPA (2003A). The showering inhalation exposure was calculated based on assumptions of a mean concentration of chloroform in the air while showering of 190 µg/m^3; an average breathing rate of 0.67 m^3/hr; average shower duration of 0.12 hr/day (7.3 minutes) ; an inhalation absorption factor of 0.63; and mean body weight of 70 kg. The estimate of showering time includes both actual shower duration and exposure to chloroform in the bathroom air immediately following the showering activity. The calculation of dermal exposure was based on a mean chloroform concentration of 24 µg/L, dermal absorption of water 3.52x10^{-6} µg per µg/L per cm^2-min., 5 minute shower duration, and an average body surface of 290 cm^2/kg.

Diet (other than fresh or estuarine fish)

The USEPA (2003A) summarized dietary exposure to chloroform from a variety of major food items. FDEP averaged these foods into several broader categories including fruits, vegetables, total meat, dairy, grain, and (marine) fish. The food items were averaged to correspond with food categories provided in the latest edition of the United States Environmental Protection Agency's Exposure Factors Handbook (USEPA, 2011A). The estimates were based on mean contamination levels and ingestion rates (**Table 1**). The total estimated dose from dietary items, excluding fresh and estuarine fish, was 8.21 x 10^{-4} mg/kg-day. Dairy and grain products were estimated to contribute the largest intakes.

Table 1. Dietary exposures to chloroform (from USEPA, 2003A).

Food Category	Mean Concentration µg/g	Ingestion Rate g/kg-day	Average Daily Dose mg/kg-day
Fruits	0.010	1.6	1.6 x10^{-5}
Vegetables	0.020	2.9	5.8 x 10^{-5}
Meat	0.0486	2	9.72 x10^{-5}
Dairy	0.079	6.6	5.21 x 10^{-4}
Grain	0.045	2.6	1.17 x 10^{-4}
Marine Fish	0.052	0.22	1.1 x 10^{-5}
Total			8.21 x 10^{-4}

Ambient Exposure Sources

Staples *et al.*, (1985) summarized priority pollutant concentrations in the United States using the STORET Database. They reported a median chloroform (trichlormethane) concentration of 0.3 µg/L based on 11,928 samples with a 64% detection rate. Staples *et al*., (1985) additionally reported median sediment and biota tissue concentrations of <5.0 µg/kg and 0.032 mg/kg, respectively. Ambient surface water data were queried from the IWR Run 47 database and the range of measured concentrations over the ten-year period from 2002-2011 were summarized (n=420). The mean concentration for Florida surface waters is 0.22 µg/L with 10th and 90th percentiles of 0.03 and 0.3 µg/L, respectively. The maximum observed concentration was 2.0 µg/L.

RSC Calculation

The exposure estimates described above were used to estimate a total non-surface water exposure dose of 2.11 x 10^{-3} mg/kg-day, as summarized below in **Table 2**.

Table 2. Estimated average daily chloroform exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure

	(mg/kg-day)
Inhalation of Air:	
Indoor air inhalation	3.5×10^{-4}
Outdoor air inhalation	4.0×10^{-5}
Inhalation while showering	3.2×10^{-4}
Treated drinking water ingestion	6.86×10^{-4}
Diet	8.2×10^{-4}
Dermal during showering	1.2×10^{-4}
Estimated total daily dose	2.34×10^{-3}

The reference dose (RfD) for chloroform is 0.01 mg/kg-day (USEPA, 2013C). The total non-ambient water exposure (2.34×10^{-3}mg/kg-day) accounts for 23.4% of the RfD. The remaining 76.6% of the RfD is available for allocation to surface water exposure routes; that is, the consumption of fresh and estuarine fish and ingestion of ambient water. Thus, an RSC value of 0.76 is suggested to be protective of human health and representative of chloroform exposures received through non-ambient sources.

1,2-Dichlorobenzene

Background

1,2-Dichlorobenzene (CASRN 95-50-1) is an anthropogenically-produced chemical that possesses a pale yellow color and exists in a liquid state at room temperature. 1,2-Dichlorobenzene is primarily used as a chemical intermediate, solvent for waxes, gums, resins, tars, rubbers, oils and asphalts, a degreaser for metals, component of deodorizers for garbage and sewage applications, as a constituent of a variety of herbicides such as diuron, and as an insecticide/fumigant used in the control of peach tree borers, bark beetles, grubs, and termites (ATSDR, 2006; OEHHA, 1997)

The primary route of exposure to 1,2-dichlorobenzene for the general population is through inhalation, although exposure can also occur through ingestion of contaminated foods and drinking water. According to the ATSDR (2006), volatilization, sorption, biodegradation, and bioaccumulation are potentially competing environmental processes and notes that the dominant fate of 1,2-dichlorobenzene is often determined by local/site-specific environmental conditions. According to the Hazardous Substances Data Bank (HSDB; No. 521), high log octanol-water partition coefficient (log Kow) values of 3.43–3.53 suggest that dichlorobenzenes have a moderate to high potential for bioaccumulation.

Exposure Source Determinations

Manufacturing and release

1,2-Dichlorobenzes are released to the environment through anthropogenic activities. One of the main estimated sources of release is through the production and use of 1,2-dichlorobenzene-based insecticides and herbicides. In addition, 1,2-dichlorobenzene is produced in large quantities as a by-product during the production of 1,4-dichlorobenzene and can be released into the environment

during the disposal of unused supplies (ATSDR, 2006). Production of 1,2-dichlorobenzene has been subject to fluctuation since the mid-1980s. In 2002, companies reported production within the range of <10 million pounds to 50 million pounds (<5,000–23,000 metric tons) (ATSDR, 2006). As of 2005, 1,4-dichlorobenzene and 1,2-dichlorobenzene were currently produced by 2 companies in the United States at 2 different locations: Solutia Inc., in Sauget, Illinois and PPG Industries, Inc., in Natrium, West Virginia (SRI, 2005).

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[5] of 1,2-dichlorobenzene in 2011 accounted for 49,193.21 pounds with the majority of release/disposal occurring through point source air emissions and fugitive air emissions. (TRI2011, 2013A). Total reported off-site disposal or other releases[6] in 2011 accounted for 431 pounds of 1,2-dichlorobenzene with the majority of disposal/release occurring through "other off-site management" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for 1,2-dichlorobenzene in 2011 was 49,624.21 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 53,548.35 pounds of 1,2-dichlorobenzene with the majority of disposal/release occurring through point source emissions and fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 4,747.05 pounds of 1,2-dichlorobenzene with the majority of disposal/release occurring through landfill-based disposal (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for 1,2-dichlorobenzene in 2012 was 58,295.40 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

1,2-Dichlorobenzene has been detected at trace levels in drinking waters. An investigation conducted by Oliver *et al.* (1982) to assess chlorobenzene concentrations in various environmental

[5] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[6] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

media and biota originating from the Great Lakes region revealed a mean 1,2-dichlorobenzene concentration of 0.003 ppb detected in drinking water samples from 3 cities near Lake Ontario in 1980. According to a preliminary assessment conducted by the United States Environmental Protection Agency (1975), a concentration of 1 ppb was detected in Miami, FL drinking water and qualitative detections were reported for Philadelphia, PA and Cincinnati, OH. A maximum contaminant level (MCL) of 0.6 mg/L has been established by the United States Environmental Protection Agency for 1,2-dichlorobenzene (USEPA, 2009D).

1,2-Dichlorobenzene is regulated as a VOC in drinking water and all non-purchased community water systems (CWSs) and non-transient non-community water systems (NTNCWSs) are required to sample for VOCs (USEPA, 2009C). In the *Contaminant Occurrence Support Document for Category 2 Contaminants for the Second Six- Year Review of National Primary Drinking Water Regulations,* the United States Environmental Protection Agency analyzed the reported VOC data from 49,969 public water systems (PWSs) during the period from 1998 to 2005 (USEPA, 2009C). For drinking water originating from ground water sources, a median concentration of 0.9 μg/L and a 90th percentile concentration of 3 μg/L were detected (USEPA, 2009C). For drinking water originating from surface water sources, a median concentration of 0.5 μg/L and a 90th percentile concentration of 1.3 μg/L were detected (USEPA, 2009C).

For the purposes of RSC calculation, the MCL of 0.6 mg/L was utilized because it represents the most conservative estimate of general population exposure through the ingestion of drinking water. In addition, a standard drinking water intake rate of 2.0 L/day and a standard body weight of 70 kg were also used in the calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of 1,2-dichlorobenzene received through the consumption of drinking water was 0.0171 mg/kg-day.

Air

Although inhalation is considered the main exposure route for 1,2-dichlorobenzene, ambient and indoor air concentrations are minimal when compared to 1,4-dichlorobenzene. According to the ATSDR (2006), indoor inhalation of 1,2- or 1,3-dichlorobenzene is not expected to be a significant route of exposure due to the fact that these chemicals are not as prevalently detected in household and consumer products as 1,4-dichlorobenzene. 1,2-Dichlorobenzene concentrations in ambient outdoor air typically range from 0.01 to 0.1 ppb (ATSDR, 2006). According to an atmospheric VOC assessment conducted by Brodzinsky and Singh (1982), the mean 1,2-dichlorobenzene concentrations from 226 source-dominant points and 674 urban/suburban points in the United States have been reported to be 200 and 56 parts per trillion, respectively. Wallace *et al.* (1989), reported that 1,2-dichlorobenzene was detected at median concentrations ranging from 0.1-2.2 $\mu g/m^3$ in homes in the United States. Field *et al.* (1992) reported an indoor air 1,2-dichlorobenzene concentration of 1.4 $x10^{-4}$ ppm. Indoor air concentrations of 1,2-dichlorobenzene have also been shown to seasonally fluctuate. Pellizzari *et al.* (1986) reported an indoor residence-based 1,2-dichlorobenzene concentration of 3.48 x 10^{-6}ppm during the summer and an indoor residence-based 1,2-dichlorobenzene concentration of 1.39 $x10^{-5}$ ppm during the winter. The ATSDR (2006) reports that the average daily adult respiratory exposure to 1,2-dichlorobenzene is approximately

1.8 µg. For the purposes of RSC calculation, the average daily adult respiratory exposure value of 1.8 µg/day was used. A standard body weight of 70 kg was also used to calculate dose (USEPA, 1997). The resultant estimated average daily dose of 1,2-dichlorobenzene received through inhalation was 2.57 $x10^{-5}$ mg/kg-day.

Groundwater

Through a collaborative partnership between the USGS and the United States Environmental Protection Agency, national water quality assessment (NWQA) data from the years ranging from 1992-2001 were analyzed for their 1,2-dichlorobenzene content. For groundwaters, a total of 4,660 samples were taken from 4,159 sites of which 0.6% of samples detected 1,2-dichlorobenzene representing 0.7% of the sites under analysis (USEPA, 2009C). A median 1,2-dichlorobenzene concentration of 0.036 µg/L and a 99th percentile 1,2-dichlorobenzene concentration of 1.502 µg/L were produced from the groundwater samples under analysis (USEPA, 2009C).

Oceanic/marine concentrations

Information concerning oceanic/marine concentrations of 1,2-dichlorobenzene could not be located.

Soil/sediment

Information and data concerning 1,2-dichlorobenzene concentrations in typical soils are scarce. According to Wang *et al.* (1995), chlorobenzene levels in uncontaminated soils are generally less than 0.4 mg/kg for dichlorobenzene congeners and less than 0.1 mg/kg for other chlorobenzene congeners. Biodegradation by a number of distinct soil microbial species does have the capacity to decrease 1,2-dichlorobenzene concentrations under aerobic conditions. Sorption to soils with a greater organic content negatively influences the ability of 1,2-dichlorobenzene to volatilize. Application of sewage sludge possesses the capacity to increase concentrations of 1,2-dichlorobenzene in soils (ATSDR, 2006). The Florida Department of Environmental Protection has established a residential (direct exposure) soil clean-up target level of 880 mg/kg as per Chapter 62-777, F.A.C. (FDEP, 2005). For the purposes of RSC calculation, a soil concentration of 0.40 mg/kg was utilized. In addition, a standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also used (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of 1,2-dichlorobenzene received through soil ingestion was 2.86 $x10^{-7}$ mg/kg-day.

1,2-Dichlorobenzene has also been detected in sediments. According to Oliver *et al.* (1982), mean 1,2-dichlorobenzene concentrations of 1, 8, 2, and 11 ppb were detected in the superficial sediments from Lakes Superior, Huron, Erie, and Ontario, respectively.

Diet (other than fresh or estuarine fish)

Information and data concerning 1,2-dichlorobenzene concentrations detected in different food types are very limited. The United States Food and Drug Administration conducted an analysis of pesticide residuals in specific food types through their Total Diet Study program. The information summarized in this analysis pertains to Total Diet Study market baskets 1991-3 through 2003-4 collected between September 1991 and October 2003 (USFDA, 2006). **Table 1** below displays the

food types analyzed in the total diet study that can be separated into food-based categories associated with specific intake rates found in the United States Environmental Protection Agency's 2011 Exposure Factors Handbook.

Table 1. Limited Selection of Food Types Analyzed for 1,2-Dichlorobenzene in FDA's Total Diet Study Program

Food Type	Mean Concentration (ppm)
Beef, ground, regular, pan-cooked	0.00016
Beef roast, chuck, oven-roasted	0.00027
Frankfurter (beef/pork), boiled	0.00005
Bologna (beef/pork)	0.00014
Fish sticks or patty, frozen, oven-cooked	0.00007
Eggs, scrambled w/ oil	0.00020
Muffin, fruit or plain	0.00091
Meatloaf, beef, homemade	0.00030
Ice cream, light, vanilla	0.00014
Crackers, graham	0.00005
Potato, french-fried, fast-food	0.00025

*As per the United States Environmental Protection Agency's 2011 Exposure Factors Handbook (Chapter 14 Total Food Intake) beverages, sugar, candy, and sweets, and nuts (and nut products) were not included because they could not be categorized into the major food groups. In addition, foods analyzed such as "Quarter-pound cheeseburger on bun, fast-food" were not included in the analysis due to the fact that they represented composite foods containing food types separately categorized into food groups.

According to an analysis conducted by Hiatt *et al.* (2004), 1,2-dichlorobenzene was detected at average concentrations of 4 x10^{-5}, 5 x10^{-5}, and 4 x10^{-5} mg/L in whole milk, 2% milk, and 1% milk, respectively. Wang *et al.* (1994) also reported 1,2-dichlorobenzene was detected in potato cores at a concentrations of 0.328 µg/kg and pea seeds at a concentration of 0.112 µg/kg. For the purpose of RSC calculation, an overall average of the food concentrations presented above was taken to estimate total intake. A standard dietary intake rate of 29 g/kg-day was used to calculate dietary exposure dose (USEPA, 2011A). An estimated average daily dose of 5.63 x10^{-6} mg/kg-day received through dietary intake was subsequently generated. To ensure that the estimated dietary exposure dose accurately represented a realistic dietary exposure scenario for the general public, an additional multiplication factor of 10 was applied providing added conservatism to this dose estimate; that is, the exposure was conservatively increased by an order of magnitude. The additional factor was used to account for the uncertainty in the estimate associated with the somewhat limited database on foods, particularly related to fruits and vegetables. Thus, with the addition of this uncertainty factor, the resultant estimated average daily dose of 1,2-dichlorobenzene received through dietary intake was 5.63 x10^{-5} mg/kg-day.

Ambient Exposure Sources

In water, the major dichlorobenzene-removal processes are likely to be adsorption onto sediments and bioaccumulation in aquatic organisms (WHO, 2003B). The United States Environmental Protection Agency conducted a concurrent analysis of NAWQA data from the years 1992-2001, for detections of 1,2-dichlorobenzene in ambient surface waters. For ambient surface waters a total of 1,419 samples were taken from 191 sites of which 3.2% of samples detected 1,2-dichlorobenzene representing 9.4% of the sites under analysis (USEPA, 2009C). A median 1,2-dichlorobenzene concentration of 0.04µg/L and a 99th percentile 1,2-dichlorobenzene concentration of 0.447µg/L were produced from the ambient surface water samples under analysis (USEPA, 2009C). According to Staples *et al.* (1985), 1,2-dichlorobenzene was detected in 0.6% of 1,077 surface water samples recorded in the STORET database at a median concentration of <10 ppb.

Due to the large bioconcentration factor and log Kow of 1,2-dichlorobenzene, it is expected that this chemical possesses the potential to bioaccumulate in aquatic biota. According to Oliver *et al.* (1982), 1,2-dichlorobenzene concentrations detected in lake and rainbow trout from the Great Lakes ranged from 0.3 to 1.0 ppb. According to the ATSDR (2006), respective 1,2-dichlorobenzene concentrations of 0.08, 0.26, 0.06, and 0.06 ppm were detected in Atlantic croakers, blue crabs, spotted sea trout, and blue catfish collected from the Calcasien River estuary.

RSC calculation

The estimated doses received through daily exposure to1,2-dichlorobenzene were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 2** below.

Table 2. Estimated average daily 1,2-dichlorobenzene exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg-day)
Inhalation of Air	2.57×10^{-5}
Soil ingestion	2.86×10^{-7}
Treated drinking Water ingestion	0.0171
Diet[1]	5.63×10^{-5}
Estimated total daily dose	0.0172

1. Includes a 10-fold conservative adjustment to account for limitations in dietary data.

The reference dose for 1,2-dichlorobenzene is 9×10^{-2} mg/kg-day (USEPA, 2013C). The estimated total non-ambient exposure 0.0172 mg/kg-day represents 19.1% of the RfD. The remaining 80.9% is available for allocation to surface water exposures through routes such as estuarine fish consumption. Thus, a chemical specific RSC of 0.80 is suggested to be protective of human health and representative of 1,2-dichlorobenzene exposures received through ambient sources.

Endrin and Endrin Aldehyde

Background

Endrin (CASRN 72-20-8) is a solid, white, almost odorless substance that was used as an insecticide, rodenticide, and avicide (OEHHA, 1999A; ATSDR, 1996B). Production and sale of endrin for use by the general public in the United States has not occurred since 1986. Little is known about the properties of endrin aldehyde (an impurity and breakdown product of endrin) or endrin ketone (a product of endrin when it is exposed to light) (ATSDR, 1996B). No studies specific to the environmental fate of endrin aldehyde or endrin ketone could be found in the available literature. Limited information on the physical and/or chemical properties of endrin aldehyde indicates that it is highly insoluble in water (USEPA, 1981), highly immobile in soil, and will not volatilize significantly from water or soil. Any endrin aldehyde in air should exist predominantly in the adsorbed phase (Eisenreich *et al.,* 1981). Atmospheric endrin aldehyde will be transported to soil and surface water via wet and dry deposition of associated particles. Endrin aldehyde may react with photochemically generated hydroxyl radicals in the atmosphere, with an estimated half-life of 3.6 hours (SRC, 1995). In water, adsorption to sediments and bioconcentration are likely to be significant transport processes. Neither hydrolysis nor oxidation (via peroxy radicals or singlet oxygen) of endrin aldehyde is expected to be significant in aquatic systems (USEPA 1979, 1981). The estimated half-life for endrin aldehyde is more than four years (USEPA, 1979). Neither hydrolysis nor oxidation is expected to be a significant transformation process for endrin aldehyde in soil. No information could be found on the biodegradation of endrin aldehyde in aquatic systems, sediment, or soil.

Information on current levels of endrin in the environment is limited; however, the available data indicate that concentrations in all environmental media are generally negligible or below levels of concern (ATSDR, 1996B). The FDA has concluded that endrin is no longer present in the environment to the extent that it may be contaminating food or feed at levels of regulatory concern (USDA, 1995). No information could be found in the available literature on levels of endrin aldehyde or endrin ketone in the environment. The main sources for potential human exposure to endrin are residues on imported food items, unused stocks, unregistered use, inappropriate disposal, and hazardous waste sites (ATSDR, 1996B); however, there is no current evidence of significant exposures from any of these sources. Furthermore, it should be noted that in environmental media, especially in contaminated soils and sediments, the amount of endrin chemically identified by analysis is not necessarily the amount that is toxicologically available.

Exposure Source Determinations

Manufacturing and Release

According to the ATSDR (1996B), sales of endrin in the United States were estimated at 2.345 million kg (5.1-9.9 million pounds) in 1962, while less than 450,000 kg (990,000 pounds) were produced in 1971. Information on endrin could not be retrieved from the Toxic Release Inventory (TRI) database due to the fact that facilities are not required to report endrin-related releases. According to the ATSDR (1996B), the use of endrin ended in the mid-1980s and consequently, there are no longer any significant releases of endrin (and its breakdown product, endrin aldehyde) to the environment in the United States.

Non-ambient Exposure Sources

Treated drinking water

Data and/or information concerning current endrin aldehyde residues in treated drinking water samples could not be located. However, exposure to endrin and endrin aldehyde through the drinking water exposure pathway is considered negligible due to the fact that use of the parent compound, endrin, has been discontinued since the 1980's.

Air

Endrin aldehyde is a minor impurity of the pesticide endrin which is no longer produced. Production and use of endrin may have resulted in endrin aldehyde's release to the environment. This potential release could have resulted from direct release to the environment, through direct release of endrin, or from various production-related endrin waste streams. If released to air, an estimated vapor pressure of 2.0 $x10^{-7}$ mm Hg at 25° C indicates endrin aldehyde will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase endrin aldehyde will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 3.8 hours. Particulate-phase endrin aldehyde will be removed from the atmosphere by wet and dry deposition. Current data on ambient air concentrations containing endrin or any of its breakdown products could not be located. According to the ATSDR (1996B), during extensive agricultural use, 33% of the applied endrin was found to volatilize within 11 days, after which time further evaporation ceased. Thus, exposure to endrin and endrin aldehyde through inhalation of ambient air is considered negligible due to the fact that use of the parent compound was discontinued in the 1980s.

Soil

If released to soil, endrin aldehyde is expected to have slight mobility based upon an estimated Koc of 4,300. According to the ATSDR (1996B), a conservative estimate of its half-disappearance time in sandy loam soils is approximately 14 years. Therefore, the exposure risks from endrin to the general population of the United States are likely to steadily decrease over time. Note that endrin aldehyde concentrations (a breakdown product) are expected to be significantly lower (perhaps an order of magnitude) than endrin itself. According to Nash (1983), endrin has been found to volatilize significantly (20-30%) from soils within days after application. Volatilization from moist soil surfaces is expected to be slower than other soil types based upon an estimated Henry's Law constant of $4.2X10^{-6}$ atm-cu m/mole. Because endrin has not been in use for many years, this exposure route is no longer significant in the state of Florida. Endrin aldehyde is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Sherblom *et al.* (1995) analyzed sediment from nine sites in Sarasota Bay for endrin, as well as other organic contaminants. Endrin was less than either the detection limit or the quantification limit at all sites sampled, although endrin was found in one of three replicate samples from Hudson Bayou at a level of 1 ng/g, while endrin was below the detection limit or quantification limit in the other two replicates from this site. Thus, exposure to endrin and endrin aldehyde through the soil ingestion pathway is considered negligible.

Diet (other than fresh or estuarine fish)

Oral exposure to endrin and endrin aldehyde through food-based consumption is considered to be a negligible route due to the discontinued agricultural use of this product. According to the ATSDR (1996B), no endrin was detected in food samples from a Texas survey and only 0.084% of over 13,000 food samples were found to contain endrin in 1989 after cancellation of endrin use. Moreover, a study conducted by the U.S. Food and Drug Administration in 1991 revealed endrin was found in less than 1% of all food sampled (ATSDR, 1996B). Significant accumulation of endrin in the human body has not been documented to occur after exposure (IPCS, 1991A).

Ambient Exposure Sources

During the period when endrin was utilized, the most prominent route of contamination of surface water was run-off from soil (WHO working group, 1992). Volatilization from water surfaces is not expected to be an important fate process based upon this compound's Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 17 days and 132 days, respectively. However, volatilization from water surfaces is expected to be attenuated by adsorption to suspended solids and sediment in the water column. The estimated volatilization half-life from a model pond is 540 months if adsorption is considered. An estimated BCF of 5,000 suggests the potential for bioconcentration in aquatic organisms is very high. According to the OEHHA (1999A), maximum endrin concentrations in whole fish in the United States for the periods 1976-77, 1978-79, 1980-1981, and 1984 were 0.4, 0.11, 0.30 and 0.22 ppm, respectively with corresponding geometric means less than 0.01 ppm. The United States Environmental Protection Agency reviewed the National Coastal Assessment (NCA) Fish Tissue Survey Data from 1997-2000 which analyzed data from 653 estuary sites throughout the United States in their 2008 report on the environment. Analysis of this data revealed that coastal fish tissue contaminant concentrations for endrin were below EPA's guideline ranges (0.35-0.70 ppm) for all fish sampled in the NCA (US EPA, 2008A). Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions.

RSC Calculation

EPA used a default RSC value of 20 percent for endrin based on a recommendation from EPA's drinking water program. Oregon DEQ proposed criteria for endrin using a RSC value of 80 percent (Matzke *et al.*, 2011), which is an RSC value that Florida DEP supports. Likewise, FDEP does not anticipate exposure to endrin aldehyde from means other than water and fish ingestion and therefore, proposes to use a RSC of 0.8 for the parameter. This is consistent with EPA guidance, which states using a default RSC Percentage Floor Value of 20% and a Ceiling of 80% (USEPA, 2000B).

EPA has recommended using the 20% RSC default when routes of water exposures other than oral or sources of exposure other than fish and water **are anticipated**, but adequate data are lacking to quantify those exposures. EPA guidance states that if it can be demonstrated that other sources and routes of exposure **are not anticipated** for the chemical in question (based on information about its known/anticipated uses and chemical/physical properties), then the 80% ceiling is

recommended. This 80% ceiling is a way to provide adequate protection for those who experience exposures (from any or several sources) higher than available data may indicate. As seen in this discussion, FDEP has strong evidence that exposure to endrin aldehyde is expected to be negligible. Thus, an RSC of 0.80 for both endrin and endrin aldehyde is proposed to be protective of the general population with respect to ambient exposures. This value is likely to be highly conservative given that the parent compound has been banned for a considerable time.

Methyl Bromide (Bromomethane)

Background

Methyl bromide (CASRN 74-83-9) is an odorless, colorless gas that has been used as a soil fumigant and structural fumigant to control pests across a wide range of agricultural sectors. Soil fumigation was the primary use of methyl bromide in the U.S and accounted for approximately 65% of total use (ATSDR, 1992), estimated at 25,500 metric tons (56 million pounds) at the height of use in 1991 (USEPA, 2013E). Historical use of leaded gasoline with bromine-containing additives also resulted in the release of methyl bromide in automotive exhaust fumes, although current releases from exhaust fumes are estimated to be much lower.

Because methyl bromide depletes the stratospheric ozone layer, the amount produced and imported in the United States was reduced incrementally until it was phased out on January 1st, 2005, pursuant to obligations under the Montreal Protocol on Substances that Deplete the Ozone Layer (Protocol) and the Clean Air Act (CAA). Critical use exemptions (CUEs) are permitted under Section 604(d) of the Clean Air Act and the Montreal Protocol on Substances that Deplete the Ozone Layer. Each year, EPA solicits applications for CUEs from methyl bromide users. The U.S. Government, after reviewing the applications, seeks authorization for those uses from the Parties to the Montreal Protocol. Once the Parties authorize an amount of methyl bromide for those critical uses, EPA publishes a rule allowing for the production of critical use methyl bromide. Annual methyl bromide exemptions are summarized in **Table 1**.

Table 1. 2005-2014 Critical Use Exemption Authorizations. Amount authorized is based on a 1991 baseline level.

Calendar Year	Amount Nominated (percent of baseline)	Amount Authorized (percent of baseline)
2005	39	37
2006	35	32
2007	29	26
2008	23	21
2009	19.5	16.7
2010	13.4	12.7
2011	9.4	8.1
2012	4.6	4.0
2013	2.5	2.2

Calendar Year	Amount Nominated (percent of baseline)	Amount Authorized (percent of baseline)
2014	1.7	1.7
2015	1.5	To be determined

Methyl bromide is not persistent in soil due to rapid evaporation, with a soil half-life ranging from 0.2 to 0.5 days depending on depth (Jury *et al.*, 1984). Methyl bromide is soluble in water and is present at low concentrations in ocean waters, likely due to natural production by marine organisms (IARC, 1986). However, due to rapid volatilization, the half-life in water is estimated to be on the order of hours to days depending on depth, temperature, and mixing (USEPA, 1986). Additionally, due to its low octanol/water partition coefficient (Kow), methyl bromide is not expected to bioaccumulate in aquatic organisms; the estimated bioconcentration factor is approximately 3 (ATSDR, 1993).

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[7] of methyl bromide in 2011 accounted for 307,749.12 pounds with the majority of release/disposal occurring through point source air emissions, fugitive air emissions, and underground injection into Class I wells. (TRI2011, 2013A). Total reported off-site disposal or other releases[8] in 2011 accounted for 23 pounds of methyl bromide with the majority of disposal/release occurring through RCRA Subtitle C Landfill-based disposal (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for methyl bromide in 2011 was 307,772.12 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 189,200.43 pounds of methyl bromide with the majority of disposal/release occurring through point source emissions and fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 10.61 pounds of

[7] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[8] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

methyl bromide with the majority of disposal/release occurring through RCRA Subtitle C landfill-based disposal (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for methyl bromide in 2012 was 189,211.04 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Air

Methyl bromide concentrations in air are available from several sources and range from 0.002- 5.1 $\mu g/m^3$ in rural, suburban, and urban air in the United States in the 1970s and 1980s (Table 5-2; ATSDR, 1992). The highest mean concentration reported was 2.2 $\mu g/m^3$ for urban air, and this value was selected to represent air concentrations for the RSC calculation. A standard inhalation rate of 16 m^3/day and body weight of 70 kg (USEPA 2011A; USEPA 1997) were used to generate an inhalation dose of 5.03 $x10^{-4}$ mg/kg-day. This air exposure estimate is assumed to be conservative, as it is the highest reported mean concentration and includes inputs from leaded gasoline, which has subsequently been phased out across the entire United States.

Treated drinking water

Methyl bromide concentrations in drinking water are low. In municipally-supplied water, methyl bromide is an assumed chlorination by-product; however, only trace concentrations are detected in tap water (ATSDR, 1992). It was detected in groundwater near two of 450 hazardous waste sites where it was investigated (CLSPD, 1989) with a geometric mean concentration of 17 µg/L; however, methyl bromide was not detected above 1 ppb in drinking water supply wells (Lim, 2002). The drinking well detection limit of 1 µg/L for groundwater was used to estimate an exposure through drinking water of 0.000029 mg/kg-day, assuming a water consumption rate of 2.0 L/day for a 70 kg adult (NRC, 1977; USEPA 1997). This drinking water exposure is assumed to be conservative, as it assumes a methyl bromide tap water concentration equal to the detection limit, whereas drinking water supply wells and most wells do not likely contain detectable concentrations of methyl bromide.

Oceanic/marine concentrations

In ocean waters, concentrations ranging from 1 to 2 ng/L are typically reported (Lovelock, 1975; Singh *et al.,* 1983b). Based on its low log K_{ow} value, methyl bromide is not expected to significantly bioconcentrate. However, to conservatively estimate methyl bromide concentrations in ocean fish tissue, a bioconcentration factor of 3.75 was multiplied by an ocean water concentration of 2 ng/L, resulting in an estimated ocean fish tissue concentration of 7.5 ng/kg. A marine fish consumption rate of 0.22 g/kg-day was conservatively assumed. The resulting fish ingestion exposure estimate is 1.65×10^{-9} mg/kg-day and assumes all fish eaten are deep water ocean fish.

Soil

In soil, methyl bromide was not detected in any of the 455 hazardous waste sites where it was investigated (CLPSD, 1989). Due to rapid volatilization in soils, exposure via contact with soils and sediment is expected to be negligible (ATSDR, 1993; Lim, 2002).

Diet (other than fresh or estuarine fish)

In food, methyl bromide residues ranged from below the detection limit to about 15 ppm, with the highest residues associated with nuts and nut-based products. Tissue residue data were provided to USEPA by the Methyl Bromide Industry Panel for over 230 commodities and their food forms (*i.e.,* raw, baked, frozen, cooked). Lim (2002) used these data to estimate chronic dietary exposure for the US population of 0.000127 mg/kg-day using consumption data from the Nationwide Food Consumption Survey (USDA, 1989-1991; cited in Lim 2002).

Ambient Exposure Sources

Methyl bromide was not detected in surface waters near any of 405 waste sites where it was investigated, and is not a common contaminant in fresh waters of the United States (ATSDR, 1992). Some methyl bromide may leach from fumigated soil into surface water (USEPA, 1986; IARC, 1986); however, most of this would be expected to quickly volatilize into air. Concentrations due to surface water exposures (either consumption of water or fish) were not estimated, but are assumed to be low based on available data. Ambient surface water data were queried from the IWR Run 47 database and the range of measured concentrations over the ten-year period from 2002-2011 were summarized (n=379). The mean concentration for Florida surface waters is 0.50 µg/L with 10th and 90th percentiles of 0.25 and 0.82 µg/L, respectively. The maximum observed concentration was 1.3 µg/L.

RSC Calculation

The exposure estimates described above were used to estimate a total non-surface water exposure dose of 6.6×10^{-4} mg/kg-day, as summarized below in **Table 2**.

Table 2. Estimated average daily methyl bromide exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg-day)
Inhalation of air	5.03×10^{-4}
Soil ingestion	Negligible
Treated drinking water ingestion	2.9×10^{-5}
Diet	1.3×10^{-4}
Marin fish	1.65×10^{-9}
Estimated total daily dose	**6.6×10^{-4}**

The total non-surface water exposure dose accounts for 47% of the methyl bromide RfD of 1.4 $x10^{-3}$ mg/kg-day (USEPA, 2013C). Therefore, surface water sources can be allotted the remainder of the allowable exposure dose, resulting in a chemical-specific RSC of 0.53, or 53%.

The chemical-specific RSC calculated for methyl bromide is likely very conservative, as exposure estimates for inhalation and in food residues do not account for recent decreases in the use of this compound and are based on maximum or upper percentile concentrations likely measured when the methyl bromide was in wider use. Beginning in 1992, use of methyl bromide was phased out in the U.S. to reduce stratospheric ozone layer depletion. In 2005, methyl bromide use was ended except for allowable critical use exemptions. These exempt uses accounted for just 1,022,826 kg in 2012 (4% of the 1991 use baseline). Thus, the exposure estimates presented above for non-surface water sources are an overestimate. As current non-surface water exposures are likely a fraction of those estimated herein, an RSC for methyl bromide based on only recent environmental concentration data would be greater than 0.53, likely substantially so. Use of this RSC value is therefore highly protective.

Di-*n*-Butyl Phthalate

Background

Di-*n*-butyl phthalate (DBP; CASRN 84-74-2) is a phthalate ester used as a plasticizer. It is found in many common consumer products including home furnishings, paints, clothing, and cosmetics. It is widespread in the environment because of its many uses, and has been identified at low levels in all environmental media. Exposure of the general population to DBP may occur through contact with contaminated air, water, food, soil, and/or products which contain di-*n*-butyl phthalate (ATSDR, 2001).

In air, di-*n*-butyl phthalate may be adsorbed to particulate matter or occur as a vapor. It is expected to decompose in air, or be transported to water and/or soil by wet (snow or rain) or dry (wind and settling) deposition (ATSDR, 2001). It is taken up by a variety of aquatic organisms (ATSDR, 2001). In water and soil, it is subject to microbial degradation; both aerobic and anaerobic degradation have been reported (ATSDR, 2001). Di-*n*-butyl phthalate is expected to have limited mobility in soil based on a reported Log K_{oc} of 3.14 (Russell and McDuffie, 1986) and also, 4.17 (Sullivan *et al*., 1982).

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[9] of di-n-butyl phthalate in 2011

[9] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not

accounted for 170,474.26 pounds with the majority of release/disposal occurring through underground injection to Class I wells and point source air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[10] in 2011 accounted for 11,385.56 pounds of di-n-butyl phthalate with the majority of disposal/release occurring through landfill-based disposal and waste brokers (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for di-n-butyl phthalate in 2011 was 181,859.83 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 40,114.80 pounds of di-n-butyl phthalate with the majority of disposal/release occurring through underground injection to Class I wells and fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 13,693.76 pounds di-n-butyl phthalate with the majority of disposal/release occurring through RCRA Subtitle C landfill-based disposal and disposal to other landfills (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for di-n-butyl phthalate in 2012 was 164,774.56 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Air

Di-*n*-butyl phthalates in outdoor air have been recorded at concentrations ranging from 2.3 x 10^{-7} to 4.99 x 10^{-5} mg/m^3 in Sweden and the United States (Thurén and Larsson, 1990) and Canada (Otson *et al.*, 1991). Concentrations over New York City were measured at 3.2 x 10^{-6} to 5.7 x 10^{-6} mg/m^3 (Bove *et al.,* 1978), and in industrialized areas along the Niagara River at 6.2 x 10^{-6} mg/m^3 in particulate matter and 4.5x10^{-6} mg/m^3 as vapor (Hoff and Chan, 1987). Concentrations of di-*n*-butyl phthalate in indoor air in Canada was measured at >1.0x10^{-5}mg/m^3 (Otson *et al.*, 1991). Estimated daily intake of DBP from indoor air by the Canadian population ranged from 0.68 to1.1 µg/kg body weight/day (Chan and Meek, 1994). Compared to the exposure calculated for just outdoor air as part of the same study (0.00021-0.00041 µg/kg body weight/day), the contribution of DBP from outdoor air is likely negligible. For the purposes of RSC calculation, 1.06 and 0.012 mg/m^3 were used as estimates of concentrations found in indoor and outdoor air, respectively, which originate from the Clark *et al.* (2011) analysis. The values were taken from the American Chemistry Council database and represent the most conservative measurements found in the

authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[10] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

literature. An indoor inhalation rate of 12.878 m^3/day, an outdoor inhalation rate of 3.122 m^3/day, and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DBP received through indoor inhalation exposures was 1.95 $x10^{-4}$ mg/kg-day and the resultant estimated average daily dose of DBP received through inhalation of outdoor air was 5.35 x 10^{-7} mg/kg-day.

Treated drinking water

In Keith *et al.* (1976), DBP was detected in drinking water in 6 of 10 city water supplies at concentrations ranging from 0.1- 0.2 µg/L, while the concentration from one city was measured at 5.0 µg/L. It should be noted that from 1988-2011, 4,480,085 pounds of DBP have been released to underground injection wells by Ascend Performance Materials in northwest Florida (TRI2011, 2013A). This release continued through 2011, with 135,406 pounds released to injection wells that year. For the purpose of RSC calculation, a DBP concentration of 0.2 µg/L was utilized due to the fact that this value represents the most conservative estimate of exposure to DBP received through drinking water that could be located. A standard water ingestion rate of 2.0 L/day and a standard body weight of 70 kg were also utilized (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of DBP received through the ingestion of drinking water was 5.71 x 10^{-6} mg/kg-day.

Oceanic/marine concentrations

No information could be located on the concentrations found in or exposure from marine waters.

Soil and dust

DBP rapidly degrades in soil and sediments (ATSDR, 2001; Staples *et al.*, 1997). A concentration of 500 µg/L was found to take 1-5 days to degrade to one-half the initial concentration (ATSDR, 2001; USEPA, 1984). DBP in four different soil types was shown to degrade by greater than 80% within 80 days in nearly every case (ATSDR, 2001; Inman *et al*., 1984). Degradation has been shown to be retarded near an oil field waste water discharge. DBP was identified in 280 soil samples from the 471 NPL hazardous waste sites (ATSDR, 2001; HazDat, 2001). Concentrations ranging from <0.1 to 1.4 µg/g were found in soil from three cities in Ontario. Additionally, Clark *et al.* (2011) used a concentration of 0.011 µg/g to calculate exposure from soil. For the purposes of RSC calculation, the conservative concentration of 1.4 µg/g was used. A standard soil ingestion rate of 20 mg/day and a standard body weight of 70 kg were also utilized (U.S. EPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DBP received through soil ingestion was 4.0 $x10^{-7}$mg/kg-day.

Due to the ubiquitous nature of phthalates in consumer products, these chemicals are often detected in household dusts. Clark *et al.* (2011) reported an ingested dust DBP concentration of 132 µg/g. For the purposes of RSC calculation, the above Clark *et al.* (2011) concentration was utilized to estimate exposure. A standard dust ingestion rate of 30 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DBP received through dust ingestion was 5.66 x 10^{-5} mg/kg-day.

Diet

Based on a review of existing literature and data, the greatest risk of exposure to di-*n*-butyl phthalate is from food, specifically dairy products, fish, and seafood, if these foods comprise a large part of the diet. If dairy products, fish, and seafood are not a large part of the diet, inhalation of contaminated air is likely to present the greatest risk associated with exposure (ATSDR, 2001). DBP is an FDA-approved indirect food additive, meaning that it is used in food containers. It was found in food packaged in paper and board packing materials in the range of <0.02-62 µg/g food (ATSDR, 2001). Clark *et al.* (2011) estimated a mean exposure of 0.033 µg/g from food derived from composite diet samples. Mean concentrations for several food groups were calculated based on reported DBP levels from four sources. These mean values were used to calculate exposure to di-*n*-butyl phthalate from food (**Table 1**). A summary of each study and the assumptions made are given below the table.

Table 1. Summary of mean DBP levels in major food categories from four studies and estimated dietary exposures from each item and through overall diet.

Food Item[1]	Schecter *et al.* (2013) (µg/g)	Chan and Meek (1994) (µg/g)	ATSDR (2001) (µg/g)	Wormuth *et al.* (2006) (µg/g)	Average (µg/g)	Intake rates (g/kg-day)	Exposure (mg/kg-day)
Dairy	0.05325	1.5		0.0104	0.5212	6.6	3.44×10^{-3}
Fruit/Veggies	0.0007	0.2225		0.0117	0.0783	4.5	3.52×10^{-4}
Grain	0.0159	0.62		0.0612	0.232	2.6	6.04153×10^{-4}
Meat	0.0007			0.0123	0.0065	2	1.3033×10^{-5}
Fats	0.0035	0.64		0.025	0.223	1.2	2.67×10^{-4}
Condiments	0.0154				0.0154	0.2	3.08×10^{-6}
Fish[2]	0.011	0.5	0.2	0.001	0.178	0.22	3.916×10^{-5}
Total							$\mathbf{4.7 \times 10^{-3}}$

1. Intake rate for each food group (in g/kg-day) were taken from EPA's 2011 *Exposure Factor Handbook* as noted in the methods section, with the exception of condiments. The condiments intake rate is from Dinovi and Brookmire (2011).
2. Fish included in this dietary estimate due to the fact they are assumed not to have come from fresh or estuarine waters.

Chan and Meek (1994)

DBP was measured in 98 different foods from Canada. DBP was detected in butter, freshwater fish, cereal products, baked potatoes, coleslaw, bananas, blueberries, pineapples, margarine, white sugar, and gelatin desert. The concentrations measured in butter, margarine, cereal products, freshwater fish and the fruits/veggies were used in exposure calculations. The concentrations from coleslaw and gelatin desert were not used due to the difficulty in assigning an appropriate intake rate, and in the case of coleslaw, uncertainty in knowing what and how much of each ingredient went into making the coleslaw tested. The minimum detection limit for foods with measures of DBP below detect were not given so no concentration went into the mean calculations. The foods from

this study were placed into a group as follows: fats (butter, margarine), grain (cereal), and fruit/veggies (baked potatoes, bananas, blueberries, and pineapples).

Schecter et al. (2013)

Schecter *et al.* (2013) measured DBP in 65 foods, grouped into beverages, milk, other dairy, fish, fruits/vegetables, grain, beef, pork, poultry, meat/meat products, vegetable oils, and condiments. DBP was not detected in any of the 8 beverages tested or in any of the meats (beef, pork, poultry, meat/meat products). For the calculations described herein, milk and other dairy were grouped into a single 'dairy' category. The concentrations are means, with one-half the LOD conservatively used for measures below detect. Vegetable oils were placed in the 'fats' food category.

Wormuth et al. (2006)

Mean concentrations of DBP in food from various sources (North America, Asia, and Europe) are presented in Table IV of Wormuth *et al.* (2006). A mean concentration was calculated for each food group using the reported means. The following food categories from this study were not used due to the difficulty in assigning them to an appropriate food group: cakes/buns/puddings, bakeries/snacks, nuts/nut spreads, preserves/sugar, confectionary, spices, soups/sauces, and tea/coffee. It should be noted that DBP was not detected in milk/milk beverages, ice cream, yogurt, cheese, sausages, vegetables, preserves/sugar, juices, soups/sauces, soft drinks, beer, wine, spirits, tap water, bottled water, commercial infant food, infant formulas, and mother's milk.

ATSDR (2001)

The ATSDR (2001) provided a range of concentrations for fish from several sources of 0.078 to 0.2 µg/g. FDEP conservatively used the upper end of the range.

<u>Personal care and consumer products</u>

Several million tons of phthalates are used each year in the production of soft polyvinyl chloride and other plastics that are used in many consumer and personal care products (e.g., makeup, deodorant, perfume, nail polish). Phthalates are not chemically bound to the products they are constituents of, which subsequently promotes continuous release to ambient air and the potential for increased permeation throughout the parent consumer product. Although DBP is not among the most commonly used phthalate plasticizers, it still may be used in many manufactured goods. Thus, exposure via consumer products is a potential significant source.

Measured concentrations from indoor air would take into consideration some of the exposure from consumer products encountered by the general population. However, these indoor air estimates do not consider short-term and (likely greater) exposures associated with the direct use of consumer products. Additionally, indoor air estimates do not account for dermal or oral exposures, particularly for at-risk populations, such as children and women. Children, especially very young children, may be at a greater risk of exposure due their behavioral patterns. They drink more fluids, have a larger skin surface in proportion to their body volume, they may consume more dairy products, they crawl on the floor/ground, put things in their mouths, and/or may eat inappropriate

things (like dirt or paint chips) (ATSDR, 2001). Women, in general, may use more personal care products, such as makeup, perfume, or nail polish, than do men.

Wormuth *et al*. (2006) conducted an extensive analysis of exposure to eight phthalate esters, including DBP, for Europeans. The analysis included exposures from inhalation of indoor air, outdoor air, and while using spray paints; dermal exposure from personal care products, gloves, and textiles; and, oral exposure from food, dust, mouthing (young children) and ingestion of personal care products. They estimated daily exposures for seven age and gender groups (consumer groups): infants (0-12 months, 5.5 kg bw); toddlers (1-3 years, 13 kg bw); children (4-10 years, 27 kg bw); female adolescents (11-18 years, 57.5 kg bw); male adolescents (11-18 years, 57.5 kg bw); female adults (18-80 years, 60 kg bw); and, male adults (18-80 years, 70 kg bw). FDEP used the mean exposures for each consumer group as an additional line of evidence in evaluating the RSC for DBP. This additional line of evidence provided information on the protectiveness of the RSC calculated using the typical exposure routes (diet, inhalation, drinking water, and soil and dust ingestion), when additional potential exposure through consumer products is also considered.

Koo and Lee (2004) conducted a review of three phthalates in cosmetics available on the South Korean market. Their study included a wide range of personal care products, including perfume, nail polish, hair products, and deodorant. They estimated a mean total daily exposure to DBP from these products of 3.935 µg/kg-day (3.953 x10^{-3} mg/kg-day). The estimate was based on exposure via both dermal absorption and inhalation and was used, by FDEP, to represent personal care product exposure within the tabulation of total non-ambient exposure to DBP for purposes of RSC determination.

Ambient Exposure Sources

The National Drinking Water Contaminant Occurrence Database (NDOD), which contains data from ambient water samples, detected DBP at 2 of 15 lake/reservoir sites with a range and average concentration of 2.5-10.7 and 6.6 µg/L, respectively. In other surface waters, it was detected at 9 of 253 sites, with a range and average concentration of 0.2-150 and 17.1 µg/L, respectively (USEPA, 2000A). DeLeon *et al*. (1986) showed that concentrations of DBP along the Mississippi River are very consistent regardless of other inputs. Staples *et al*. (1997) reported that DBP degrades 50-100% aerobically within 1-28 days in both fresh and marine water, and anaerobically to over 90% within 30 days in fresh water. In the Netherlands, it was shown to degrade by greater than 90% during a river die-away test in 3 days. In fresh and estuarine waters in the U.S., half-lives ranging from 1.7 to 13 days have been reported (ATSDR, 2001).

DBP is not expected to volatilize rapidly from water to the atmosphere (Lyman, 1982). In water, it is found in both dissolved forms and adhered to suspended particles (Germain and Langlois, 1988 and Staples *et al.,* 1997). Many studies have shown that accumulation of DBP in the aquatic and terrestrial food chain is limited by biotransformation (Staples *et al.,* 1997). However, it was shown to accumulate in fish and invertebrates, in the form of the primary metabolite, mono-*n*-butyl phthalate (Sanders *et al*., 1973; Wofford *et al*., 1981). DBP has been reported in fish ranging from 78 to 200 µg/kg (Giam and Wong, 1987; Stalling *et al*., 1973; Williams, 1973). DBP was found in fish

from the Great Lakes harbors and tributaries ranging from $<2x10^{-5}$ to $3.5x10^{-2}$ µg/kg wet weight (DeVault, 1985).

RSC Calculation

FDEP tabulated estimated exposures via inhalation of air, ingestion of soil and dust, treated drinking water consumption, personal care products, and diet. The estimated exposures for each source were then used to calculate an overall total exposure for the general population to DBP of $8.90\ x10^{-3}$ mg/kg-day (**Table 2**). The calculated estimate of exposure to DBP accounts for 8.9 percent of the RfD (of 0.1 mg/kg-day).

Table 2. Estimated average daily di-n-butyl-phthalate exposure received through non-ambient sources by the general population.

Exposure Route (Non-Surface Water Sources)	**Estimated Exposure (mg/kg-day)**
Indoor air inhalation	$1.95\ x10^{-4}$
Outdoor air inhalation	$5.35\ x\ 10^{-7}$
Soil ingestion	$4.0\ x10^{-7}$
Dust ingestion	$5.66\ x\ 10^{-5}$
Treated drinking water ingestion	$5.71\ x\ 10^{-6}$
Diet	$4.7\ x\ 10^{-3}$
Personal care products	$3.935\ x\ 10^{-3}$
Estimated total daily dose	$\mathbf{8.90\ x10^{-3}}$

In addition to the exposure summarized in **Table 2**, FDEP reviewed literature reported on exposure to DBP from several large comprehensive studies. The findings of these studies are summarized below.

Chan and Meek (1994) estimated the daily intake of DBP by the Canadian population. The ranges of intake are shown by source (substrate/medium) and by age group in **Figure 1**. The study concluded that food contributed the greatest amount to daily intake. Outdoor air and soil pose a small, nearly negligible amount of exposure when compared to the other sources. The estimated daily intakes range from 1.9 to 5.0 µg/kg-day with ages 0.5-4 years having the highest risk of exposure.

Substrate/ medium[a]	Estimated intake by age groups of di-*n*-butyl phthalate (µg/kg body weight/day)				
	0–0.5 years[b]	0.5–4 years[c]	5–11 years[d]	5–19 years[e]	20–70 years[f]
Ambient air	0.00021–0.00030	0.00033–0.00040	0.00033–0.00041	0.00028–0.00038	0.00025–0.00034
Indoor air	0.68	0.91	1.1	0.87	0.78
Drinking water	0.11	0.062	0.033	0.022	0.021
Food	1.6	4.1	3.2	1.4	1.1
Soil	<0.0005–0.0070	<0.00038–0.0054	<0.00013–0.00049	<0.000035–0.00049	<0.000028–0.00040
Total estimated intake	2.4	5.0	2.3	2.3	1.9

Source: Chan and Meek 1994

[a]Mean concentrations in ambient air based on a small study in a limited region of Ontario were 4.5–6.2 ng/m^3; the maximum concentration in indoor air was 2.85 µg/m^3 based on a small and possibly unrepresentative number (n=9) of homes in Montreal; mean values were not specified. It is assumed that people generally spend 4 hours outdoors and 20 hours indoors. Di-*n*-butyl phthalate was not detected in drinking water in a regional study in Ontario (limit of detection, 1.0 µg/L); mean values in surface water and groundwater supplies in Alberta were 1.0 µg/L. Di-*n*-butyl phthalate was detected in butter (1.5 µ/g), fresh water fish (0.5 µg/g), cereal products (ranged from not detected up to 0.62 µg/g), baked potatoes (0.63 µg/g), coleslaw (0.11 µg/g), bananas (0.12 µg/g), blueberries (0.09 µg/g), and pineapples (0.05 µg/g), margarine (0.64 µg/g), white sugar (0.2 µg/g), and gelatin dessert (0.09 µg/g). The detection limits, which were not specified for individual foodstuffs, varied depending on the reagent blank values, interferences arising from coextracted food components, and the fat content of the food (range, 0.01–0.5 µg/g); the content in food stuffs in which di-*n*-butyl phthalate was not detected was considered to be 0. Calculated intakes are based upon consumptions of individual food composites for each age group in the population. The di-*n*-butyl phthalate content in the soil in urban areas of Port Credit, Oakville, and Burlington, Ontario, ranged from <0.1 to 1.4 µg/g. Available data were insufficient to estimate intake from consumer products, though cosmetics may contribute significantly to the exposure of some members of the general population in certain age groups, based on the percentage content of some products (0.1 to between 10 and 25%).
[b]Assumed to weigh 7 kg, breathe 2 m^3 air, drink 0.75 L water, and ingest 35 mg soil.
[c]Assumed to weigh 13 kg, breathe 5 m^3 air, drink 0.8 L water, and ingest 50 mg soil.
[d]Assumed to weigh 27 kg, breathe 12 m^3 air, drink 0.9 L water, and ingest 35 mg soil.
[e]Assumed to weigh 57 kg, breathe 21 m^3 air, drink 1.3 L water, and ingest 20 mg soil.
[f]Assumed to weigh 70 kg, breathe 23 m^3 air, drink 1.5 L water, and ingest 20 mg soil.

Figure 1. Estimated intake by the Canadian population taken from Chan and Meek (1994).

Clark *et al.*, (2011) compiled exposure estimates from several intake and primary metabolite studies. Intake studies use the concentrations found in each exposure medium and the intake rate of that medium to calculate a total exposure. Primary metabolite studies use measurements of the primary metabolite to extrapolate exposure to the original phthalate ester. The primary metabolite of DBP is monobutyl phthalate. Mean or median daily exposures from four intake and five primary metabolite studies, reported by Clark *et al.*, (2011), are shown in **Table 3**. The ranges given in the table are across all age groups and genders (if applicable). The intake rates used to calculate exposure are from Health and Welfare Canada (1993) and Health Canada (1995).

Clark *et al.* (2011) suggests that for the low molecular weight phthalates (like DBP), primary metabolite studies provide a better quantification of exposure. They also note that intake studies are plagued by contamination issues and require rigorous sample handling to exclude phthalate

ester contamination from sources inside and outside the analytical laboratory. They then go on to argue that these contamination issues can lead to false high values; that is, intake studies have a high likelihood of overestimating exposure. However, primary metabolite studies are not without complications. A thorough understanding of the metabolites of each phthalate ester is needed. It is also necessary to normalize urinary metabolite concentrations to a constant, like creatinine. However, creatinine concentrations can vary based upon age and gender, and maybe even race (Clark *et al.* 2011; Barr *et al*. 2005).

The mean or median exposures from intake studies summarized in Clark *et al.* (2011) range from 0.78-14 µg/kg-day with ages 0.5-4 years having the greatest risk (14 µg/kg-day). It should be noted that the researchers who published the total exposure of 14 µg/kg-day for toddlers (Clark *et al.* 2003), more recently published an updated total exposure of 3.6 µg/kg-day using different concentrations (from the American Chemistry Council) (Clark *et al.* 2011). The exposures calculated from primary metabolite studies range from 0.39-2.45 µg/kg-day. As with the intake studies, the results of the primary metabolite study show that young children (ages 11.8-16.5 months) have the greatest exposure to DBP at 2.45 µg/kg-day.

Table 3. Summary of exposure estimates given in Clark *et al.* (2011).

Study	Study Type	Geographical Area	Exposure Routes	Intake/Exposure (µg/kg-day)
Clark *et al*. (2011); update to Clark *et al*. (2003)	Intake	Various	Ingestion of food, drinking water, soil/dust; inhalation of air	0.78-3.4 (medians across five age groups; range from 0-70 y)
Clark *et al*., (2003)	Intake	Various	Ingestion of food, drinking water, soil/dust; inhalation of air	1.5-14 (medians across five age groups; range from 0-70 y)
Franco *et al*. (2007)	Intake	Various	Ingestion of food, drinking water, soil/dust; inhalation of air	2.7 (median; age 20-70 years only)
Wilson *et al*. (2003)	Intake	United States	Ingestion of food, drinking water, soil/dust; inhalation of indoor and outdoor air	1.4 (mean; age 2-5 years only)
CDC (Centers for Disease Control and Prevention) (2005); NHANES data 2001-2002	Primary metabolite	United States	-	0.39-0.71 (geo means across 4 age groups and genders; 6-20+ years)
Marsee *et al*., (2006)	Primary metabolite	United States	-	0.84 (median); pregnant women in 2000-2003

CDC (2003)(1999-2000 NHANES data)	Primary metabolite	United States	-	0.72-0.93 (geo means across age groups and genders; 6-20+ years)
Brock *et al*., (2002)	Primary metabolite	United States	-	2.45 (geo mean; age 11.8-16.5 months)
David (2000)	Primary metabolite	United States	-	1.56 (geo mean; age 20-60 years; NHANES III 1988-1994)

Based on the available data, it appears that while DBP may be found in many media (air, water, food, soil, and consumer personal care products), it is found at such low levels, that the overall exposure to the general population is minimal. FDEP calculated an estimated average daily total exposure of 5.5 µg/kg-day. Estimates from other studies, detailed above, support the calculation.

Wormuth *et al.* (2006) conducted an extensive analysis of exposure to eight phthalate esters, including DBP for European populations. The analysis included exposures from inhalation of indoor air, outdoor air, and while using spray paints; dermal exposure from personal care products, gloves, and textiles; and oral exposure from food, dust, mouthing (young children) and ingestion of personal care products. They concluded that all consumer groups experienced similar exposure patterns to DBP. Food was the dominant (40-90%) exposure route. In infants, toddlers, and children, indoor air (20-40%) and dust were also important sources. Additionally, for teenagers and female adults, personal care products accounted for an estimated 14 to 22% of the total exposure. Mean total daily exposures for seven consumer groups reported by Wormuth *et al*. (2006) are summarized in **Table 4**. Infants (<1 year) were the most highly exposed group at 7.0 µg/kg-day.

Table 4. Mean daily exposure to di-*n*-butyl phthalate in seven consumer groups taken from Wormuth *et al.* (2006).

Consumer Group	Mean Total Daily Exposure (µg/kg-day)
Infant	7.0
Toddlers	2.6
Children	1.2
Female Teen	1.3
Male Teens	1.1
Female adults	3.6
Male Adults	3.6

FDEP calculated a total exposure to DBP of 8.90 x10^{-3} mg/kg-day. Literature estimates from intake studies range from 0.78 to 14 µg/kg-day. The estimate of 14 µg/kg-day was later reduced to 3.6 µg/kg-day, as described above. Primary metabolite studies, which would account for all exposures, are consistent with FDEP's estimate of exposure; that is a total exposure less than 10 µg/L. Furthermore, the study by Wormuth *et al*. (2006), which did include consumer products, supports a conclusion that exposure for the general population is in the range of 1.1 to 9.45 µg/kg-day, consistent with FDEP's estimate. The preponderance of evidence strongly supports a conclusion that all combined non-ambient exposure routes account for less than 10% of the DBP RfD. The Department recommends an RSC for di-*n*-butyl phthalate of 0.9.

Diethyl Phthalate (DEP)

Background

Diethyl phthalate (DEP; CASRN: 84-66-2) is a phthalate ester used as a plasticizer in many consumer products including cosmetics (fragrances, hair sprays, nail polishes), time-released pharmaceuticals, insecticides, aspirin, tools, automobile parts, toothbrushes, toys, and medical treatment tubing. Because it is not part of the chain of polymers that makes up plastic, it can be easily released from the products that contain it (ATSDR, 1995A). DEP is also used as a camphor substitute, in solid rocket propellants, wetting agents, as a dye application agent, as a diluent in polysulfide dental impressions, and as a surface lubricant in food and pharmaceutical packaging and prescription drug coatings to enhance delivery (Schettler, 2006).

The greatest risk of exposure of the general population to DEP is from consumer products and contaminated foods (seafood, drinking water, and foods that become contaminated from packaging materials) (IPCS, 2003A). DEP is an anthropogenically-produced colorless liquid with a distinctly bitter taste (ATSDR, 1995A). According to the ATSDR (1995A), diethyl phthalate is considered to be lipophilic based on a log octanol water partition coefficient (Kow) ranging from 1.40 to 3.3, which could have implications for bioaccumulation in aquatic biota. According to the National Center for Biotechnology Information (2013A), diethyl phthalate is expected to exist in the vapor phase if released to the atmosphere with a half-life of approximately 4.6 days, has low mobility in soils, and adsorbs to suspended solids and sediments if released to a water body.

Exposure Source Determinations

Manufacturing and release

DEP is released to the environment through a variety of anthropogenic sources such as industrial discharge, disposal of consumer products, burning of consumer or household products containing DEP, and improperly contained landfill leachate that percolates through soils, reaches ground water, and subsequently contaminates both types of environmental media. Natural environmental cycling also plays a role in the redistribution of diethyl phthalate through evaporation from landfills containing DEP products, precipitation containing DEP that subsequently influences soil concentrations of DEP, and adherence of DEP to dust particles which are distributed throughout the environment by wind.

According to the U.S. National Library of Medicine's Toxic Release Inventory, there have not been any releases of DEP to the environment since 1994 (TRI2011, 2013A). However, the *Toxicological Profile for Diethyl Phthalate* (ATSDR, 1995) states that under the Super-fund Amendments and Reauthorization Act Section 313, releases of DEP are not required to be reported. Therefore, release of DEP into the environment could potentially still occur. Moreover, Chemical Data Reporting (CDR) information derived from EPA's Chemical Data Access Tool (USEPA, 2013F), which reports information on manufacturers (including importers), processing, and use of certain chemicals, reported that there are eight companies (four in NJ, one in MA, one in TN, one in MN, and one not reported) that produced more than 25,000 pounds of DEP in 2011. Nationwide, 5,594,535 pounds were produced in 2011 (USEPA, 2013F).

Non-ambient Exposure Sources

Treated drinking water

Concentrations of diethyl phthalate in treated drinking water are estimated to be low. According to the IPCS (2003A), diethyl phthalate concentrations ranging from 0.01 µg/L (in 6 of 10 US cities) to 1.0 µg/L (in Miami, Florida) were found in drinking-water samples from water treatment plants in the United States. According to the ATSDR (1995A), diethyl phthalate has been found in drinking water with concentrations ranging from 0.00001 to 0.0046 mg/L. Clark *et al.* (2011) reported a mean drinking water concentration of 0.12 µg/L. In 2008, the USGS conducted a reconnaissance study to determine the concentrations of targeted organic compounds in 7 water treatment plants in Miami-Dade County, Florida. The analysis found an average concentration of diethyl phthalate in finished (treated) drinking water of 2.0 µg/L (USGS, 2008). For the purposes of RSC calculation, a diethyl phthalate concentration of 2.0 µg/L was utilized to estimate average daily dose through water ingestion because it represents the most conservative mean estimate of diethyl phthalate concentrations previously detected in Florida's treated drinking water supply that could be located. A standard daily water intake rate of 2.0 L/day and a standard body weight of 70 kg were also utilized (NRC, 1977; USEPA, 1997). The resultant estimated average daily diethyl phthalate dose received through drinking water ingestion was 5.71×10^{-5} mg/kg-day.

Groundwater

Landfill leachate and improper disposal are major sources of diethyl phthalate that can potentially contaminate groundwater. As an artifact of anthropogenic contamination, a typical mean diethyl phthalate groundwater concentration could not be located. However, Stiles *et al.* (2008) reported that diethyl phthalate was detected in raw and treated New Jersey groundwater through the use of solid phase microextraction. Moreover, the ATSDR (1995A) reported that diethyl phthalate has been measured at hazardous waste sites in the groundwater at 0.0125 ppm.

Oceanic/marine concentrations

Information concerning a typical oceanic/marine concentration of diethyl phthalate could not be located. However, marine sediments in the San Luis Pass located in West Galveston Bay have been analyzed. Diethyl phthalate concentrations in marine sediments were reported at 9 ng/g dry wt., less than 2 ng/g dry wt., and 7 ng/g dry weight with a mean concentration of 5 ng/g dry weight (Murray *et al.*, 1981).

Soil and dust

Mobility of diethyl phthalate in soils is dependent on soil type. Microbial degradation of DEP has also been found to occur at varying rates. According to the ATSDR's public health statement (1995A), diethyl phthalate concentrations of 0.039 ppm have been found in soils at hazardous waste sites. Clark *et al.* (2011) reported a mean ingested soil diethyl phthalate concentration of 0.0023 µg/g. For the purposes of RSC calculation, the mean ingested soil diethyl phthalate concentration of 0.0023 µg/g was used. In addition, a soil ingestion rate of 20 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily diethyl phthalate dose received through soil ingestion was 6.57×10^{-10} mg/kg-day.

Given the extensive presence of phthalates in consumer goods, diethyl phthalate concentrations can also be detected in indoor dusts. Orecchio *et al.* (2013) analyzed the concentrations of a targeted number of phthalate esters in indoor dusts in Palermo, Italy and reported average concentrations of DEP in dusts for a number of additional countries. Mean DEP concentrations of 31 mg/kg in Palermo, Italy, 170 mg/kg in Bulgary, 2 mg/kg in Denmark, 3.1 mg/kg in Germany, 10 mg/kg in Norway, and 5 mg/kg in the United States were reported (Orecchio *et al.,* 2013). Clark *et al.* (2011) also reported a mean ingested dust diethyl phthalate concentration of 25 µg/g. For the purposes of RSC calculation, the mean ingested dust diethyl phthalate concentration of 25 µg/g was used because it represents the most conservative estimate concerning DEP dust exposures received in the United States. A dust ingestion rate of 30 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of diethyl phthalate received through the dust ingestion pathway was 1.07×10^{-5} mg/kg-day.

Diet (other than fresh/estuarine fish)

Phthalates are found in a wide variety of foodstuffs. Concentrations of these compounds within foods can also be externally influenced by the packaging surrounding each food item. Diethyl phthalate concentrations ranging from 2 to 5 ppm have been detected in packaged food (ATSDR, 1995A). Pies, crackers, and chocolate bars packaged in DEP-containing packaging where shown to contain concentrations of 1.8, 1.2, and 5.3 µg/kg DEP. Schecter *et al.* (2013), conducted an analysis of 72 different foods collected from the Albany, New York area to determine phthalate concentrations in different food groups. Food group concentrations from this study in addition to intake rates from EPA's 2011 exposure factors handbook were utilized to calculate exposure dose as a component of RSC analysis. Results of this analysis can be found in **Table 1** below.

Table 1 Estimated diethyl phthalate exposure through diet

Food Category	Mean Food Group Concentrations (ng/g whole weight)	Intake Rate (g/kg-day)	Exposure Dose (mg/kg-day)
Dairy	1.54	6.6	1.02×10^{-5}
Fruits/vegetables	0.12	4.5	5.4×10^{-7}

Grain	12.6	2.6	$3.28x10^{-5}$
Meats	2.09	2.0	$4.18x10^{-6}$
Fats	0.1	1.2	$1.2x10^{-7}$

*Concentrations utilized in calculations were adapted from Schecter, A., Lorber, M., Guo, Y., Wu, Q., Yun, S.H., Kannan, K., Hommel, M., Imran, N., Hynan, L.S., Cheng, D., Colacino, J.A., Birnbaum, L.S. (2013). Phthalate Concentrations and Dietary Exposure from Food Purchased in New York State. *Environmental Health Perspectives* 121(4): 473-479. Milk and other dairy concentrations were combined to form one dairy group, beef, pork, poultry, and meat and meat product concentrations were combined to form one meats category, fruits and vegetable concentrations were kept as a composite singular group and vegetable oils were analyzed as fats. The food concentrations listed above are means with one half the LOD conservatively used for measures below detect.

Air

Shields and Weschler (1987) conducted an investigation to analyze the concentrations of certain volatile organic compounds in New Jersey indoor and outdoor air through the use of passive sampling. Concentrations of diethyl phthalate in outdoor air were found to range from 0.40 to 0.52 $\mu g/m^3$ with a mean concentration of 0.47 $\mu g/m^3$and indoor air concentrations were found to range from 1.60 to 2.03 $\mu g/m^3$ with a mean concentration of 1.81 $\mu g/m^3$ (Shields and Weschler, 1987). Clark *et al.* (2011), reported a mean outdoor air concentration: 0.013 $\mu g/m^3$ and a mean indoor air concentration: 0.91 $\mu g/m^3$. For the purpose of RSC calculation, a mean outdoor air concentration of 0.47 $\mu g/m^3$ and a mean indoor air concentration of 1.81 $\mu g/m^3$ were used. An indoor inhalation rate of 12.878 m^3/day, an outdoor inhalation rate of 3.122 m^3/day, and a standard body weight of 70 kg were also used (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of diethyl phthalate received through indoor inhalation was $3.33x\ 10^{-4}$ mg/kg-day and the resultant estimated average daily dose of diethyl phthalate received through outdoor inhalation was $2.10\ x\ 10^{-5}$ mg/kg-day.

Cosmetics and personal care products

Individuals have the potential to be exposed to diethyl phthalate through a wide variety of consumer products, many of which are cosmetics, fragrances, and personal care products. The Institute of Medicine reported that *in vitro* testing by the Research Institute on Fragrance Materials has led to establishing a human skin steady-state absorption rate of 1.27 ± 0.11 mg/cm^2/hr (IOM, 2004). According to the IPCS (2003A), diethyl phthalate is listed as an ingredient in a variety of cosmetic formulations at concentrations ranging from <0.1% to 28.6% (97.5th percentile of use based on data from the International Fragrance Association), although most products contain less than 1% diethyl phthalate. Koo and Lee (2004) conducted an investigation that analyzed phthalate concentrations in a variety of different commonly used cosmetic products including 42 perfumes, 21 nail polishes, 31 hair products, and 8 deodorants. This analysis resulted in a reported DEP mean concentration of 3044.236 µg/ml for tested perfumes, a mean concentration of 1.585 µg/ml for tested nail polishes, a mean concentration of 3.280 µg/ml for tested hair products, and a mean concentration of 1473.154 µg/ml for tested deodorants. They estimated a total exposure to diethyl phthalate from the use of consumer care products of 24.879 µg/kg-day, based on both dermal and inhalation exposure routes. FDEP used this value in the computation of total estimated non-ambient exposure to diethyl phthalate.

Wormuth *et al.* (2006) conducted an extensive analysis of exposure to eight phthalate esters, including DEP for European populations. The analysis included exposures from inhalation of indoor air, outdoor air, and while using spray paints; dermal exposure from personal care products, gloves, and textiles; and, oral exposure from food, dust, mouthing (young children) and ingestion of personal care products. They estimated daily exposures for seven age and gender groups (consumer groups): infants (0-12 months, 5.5 kg bw); toddlers (1-3 years, 13 kg bw); children (4-10 years, 27 kg bw); male adolescents (11-18 years, 57.5 kg bw); male adolescents (11-18 years, 57.5 kg bw); female adults (18-80 years, 60 kg bw); and, male adults (18-80 years, 70 kg bw). FDEP used the mean exposures for each consumer group as an additional line of evidence in evaluating the RSC for DEP. This additional line of evidence provided information on the protectiveness of the RSC calculated using the typical exposure routes (diet, inhalation, drinking water, and soil and dust ingestion), when additional potential exposure through consumer products is also considered.

Medical Devices

DEP has been shown to leak from PVC dialysis tubing containing aqueous electrolyte solution perfused for 22-96 hours and was subsequently detected at levels ranging from 18 to 26 mg/L (ATSDR, 1995A). Additionally, tubing perfused with human blood for 8 hours showed elevated levels of DEP approximately 2-4 times greater than normal blood levels (ATSDR, 1995A).

Ambient Exposure Sources

Diethyl phthalate has shown a potential to accumulate in the tissues of certain aquatic biota. Diethyl phthalate was detected in edible fish from Wisconsin lakes and rivers at concentrations ranging from less than 0.02 mg/kg to 0.20 mg/kg (NCBI, 2013A). According to the ATSDR (1995A), fish taken from Siskiwit Lake on Isle Royale, Michigan, an area relatively undisturbed by anthropogenic influence, had relatively high concentrations of diethyl phthalate in their tissues: 0.4 µg/g for lake trout and 1.7 µg/g for whitefish. Literature indicates that diethyl phthalate concentrations in organism tissues are dependent on the animal and depuration, type of aquatic environment, and inputs to that system.

According to Kolpin *et al.* (2002), in a study conducted spanning the years from 1999 to 2000 diethyl phthalate was found in 11.1% of 54 stream samples collected from 30 states. As reported by the IPCS (2003A), a compilation of concentrations (1984–1997) of diethyl phthalate in North American and western European surface waters (USA, Canada, United Kingdom, Germany, Netherlands, Sweden), revealed geometric mean concentrations ranging from approximately 0.01 to 0.5 µg/L.

RSC Calculation

The Clark *et al.* study (2011) gives total exposures to DEP from two intake studies and several primary metabolite studies. A summary of each is shown below. Intake rates utilized to calculate exposure within this Clark *et al.* (2011) analysis were primarily sourced from Health and Welfare Canada and Health Canada. **Table 2** below is provided here solely as a secondary reference.

Table 2 Clark *et al.* (2011) Diethyl Phthalate Exposure Studies

Study	Study Type	Geographical Area	Exposure Routes	Intake/Exposure (µg/kg-day)
Clark *et al.* (2011)	Intake	Various	Ingestion of food, drinking water, dust/soil and inhalation of air	0.34-1.2 (medians across 5 age groups spanning 0-70 years of age)
Clark *et al.* (2003)	Intake	Various	Ingestion of food, drinking water, dust/soil and inhalation of air	0.2-10.6 (medians across 5 age groups spanning 0-70 years)
Calafat and McKee (2006)	Primary metabolite	United States	-	1.8-6.2 (across 3 age groups spanning 6 to >20 years)
Marsee *et al.* (2006)	Primary metabolite	United States	-	6.64 (median; pregnant women)
CDC (2003)	Primary metabolite	United States	-	1.7-5.9 (geo means across four age groups and genders)
Brock *et al.* (2002)	Primary metabolite	United States	-	6.3 (geo mean; age 11.8-16.5 months)
David (2000)	Primary metabolite	United States	-	12.34 (geo mean; age 20-60 years)
Kohn *et al.*(2000)	Primary metabolite	United States	-	12.0 (geo mean; age 20-60)

*Table adapted from Clark, K., David, R., Guinn, R., Kramarz, K.W., Lampi, M.A., and Staples, C.A. (2011). *Modeling Human Exposure to Phthalate Esters: A Comparison of Indirect and Biomonitoring Estimation Methods*. Human and Ecological Risk Assessment: An International Journal. Volume 17, Edition 4. pp. 923-965.

As described above, Wormuth *et al.* (2006) evaluated total DEP exposure in seven consumer groups. Their analysis included additional exposure from consumer and personal care products. They concluded that infants were the most highly exposed group followed by toddlers (**Table 3**). More than 80 percent of the exposure to DEP was caused by dermal application of personal care products for all consumer groups. The main products of concern were fragrances and aftershaves, deodorants, and skin creams or by incidental ingestion of personal care products. Additionally, contaminated air was another important source (30%) of DEP exposure.

Table 3. Mean daily exposure to DEP for seven consumer groups taken from Wormuth *et al.* (2006).

Consumer Group	Mean Total Daily Exposure (µg/kg-day)
Infant	3.41

Toddlers	1.58
Children	0.74
Female Teen	1.58
Male Teens	1.58
Female adults	1.47
Male Adults	1.17

The estimated doses received through daily exposure to diethyl phthalate preceding the Clark *et al.* (2011) table above were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 4**.

Table 4. Estimated average daily diethyl phthalate exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg-day)**
Indoor air inhalation	3.33×10^{-4}
Outdoor air inhalation	2.10×10^{-5}
Soil ingestion	6.57×10^{-10}
Dust ingestion	1.07×10^{-5}
Treated drinking water ingestion	5.71×10^{-5}
Diet: Fruits/vegetables	5.4×10^{-7}
Diet: Meats	4.18×10^{-6}
Diet: Dairy	1.02×10^{-5}
Diet: Grains	3.28×10^{-5}
Diet: Fats	1.2×10^{-7}
Personal care products	0.024879
Estimated total daily dose	**0.0254**

The reference dose (RfD) for diethyl phthalate is 0.8 mg/kg-day (USEPA, 2013C). The estimated total non-ambient exposure of 0.0254 mg/kg-day represents 3.2% of the RfD. The remaining 96.8% is available for allocation to surface water exposures through routes such as estuarine fish consumption. This value is supported by other studies of total exposure to DEP, including those that considered exposure to personal care and consumer products, which may not be fully represented in the total provided in **Table 4**. The most sensitive population (infants) reported by Wormuth *et al.* (2006) had a total dose of 0.0034 mg/kg-day. This dose is an order of magnitude lower than the one calculated by FDEP, suggesting that FDEP's exposure estimate is highly conservative. Thus, a chemical specific RSC of 0.96 is suggested to be protective of human health and representative of diethyl phthalate exposures received through ambient sources.

2-Chloronaphthalene

Background

2-chloronaphthalene (CASRN 91-58-7) is one of 75 congeners of chlorinated naphthalenes. Commercial products are generally mixtures of multiple congeners, and are substances that range from thin liquids to hard waxes to high melting point solids. Their main uses have been in cable insulation, wood preservation, engine oil additives, electroplating masking compounds, capacitors, refractive index testing oils, and as feedstock for dye production (IPCS, 2001B). Occupational exposure to 2-chloronaphthalene may occur through inhalation and dermal contact in workplaces where 2-chloronaphthalene is produced or used. The manufacturing of chlorinated naphthalenes (Halowax is the primary commercial product, which comes in different forms, each made up of different proportions of various polychlorinated naphthalenes) ceased in the U.S. in 1977. Polychlorinated naphthalenes (PCNs) are also no longer produced in Europe. There are no data on whether PCNs are produced in other countries (IPCS, 2001B). The current major sources of release of chlorinated naphthalenes in the environment are from waste incineration and disposal of items containing chlorinated naphthalenes to landfills (HSDB, No. 4014).

Monitoring data indicate that the general population may be exposed to 2-chloronapthalene via inhalation of ambient air, and ingestion of food and drinking water (HSDB, No. 4014). If released to air, 2-chloronapthalene will be degraded by reaction with photochemically-produced hydroxyl radicals. The half-life in air is estimated at 2.1 days. 2-chloronaphthalene is expected to have slight mobility in soil. Volatilization of 2-chloronaphthalene from moist soil surfaces is expected to be an important fate process. However, adsorption to soil is expected to attenuate volatilization. 2-chloronaphthalene is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Biodegradation half-lives were 59 and 79 days for 2-chloronaphthalene contained in a mixture of oil sludge that was added to soil columns along with nitrogen and phosphorus (HSDB, No. 4014). Volatilization from water surfaces is expected. Using Henry's Law constant and a model estimate, volatilization for a model river and model lake are 7.2 hours and 6.1 days, respectively. However, volatilization is expected to be attenuated by adsorption to suspended solids and sediment in the water column, based on the estimated soil organic carbon to water partitioning coefficient (Koc). The estimated half-life for a model lake is 38 days, taking into account the adsorption potential. The potential for bioaccumulation in aquatic organisms is very high, with a bioconcentration factor (BCF) of 4600 (HSDB, No. 4014).

Exposure Source Determinations

Manufacturing and release

Information and/or data could not be located concerning the manufacturing and environmental release of 2-chloronaphthalene.

Non-ambient Exposure Sources

Air

Information and data concerning 2-chloronaphthalene concentrations in air are scarce. A study of organic chemicals (including 2-chloronaphthalene) in ambient air in New Bedford, MA in 1982 did not detect 2-chloronaphthalene (Hunt *et al.,* 1982). Thirty-four PAHs (including 2-chloronaphthalene) were measured in ambient air around the Great Lakes in 1990, although 2-chloronaphthalene was not detected (Foster *et al,* 1991). According to Harner *et al.* (1997) mean atmospheric PCN concentrations at an urban site (Chicago, USA) and a semi-urban site (Toronto,

Canada) were 68 and 17 pg/m^3, respectively. In the past, 2-chloronaphthalene has also been detected at industrial sites and as a component of industrial by-products. For example, 2-chloronaphthalene has been detected in fly ash from municipal incinerators in the United States at levels up to 3 µg/kg and a concentration of up to 19.6 µg 2-chloronaphthalene/m^3 was detected at the scrubber inlet during incineration of sewage sludge (corresponding to an emission of 0.0011 kg/hr), but no 2-chloronaphthalene was detected in the scrubber outlet gases (IPCS, 2001B). For the purposes of calculating inhalation exposure for RSC determination, the mean atmospheric value of 68 pg/m^3 was utilized due to the fact that this value was the most conservative estimate that could be located. A standard inhalation rate of 16 m^3/day and a standard body weight of 70 kg were also used to calculate dose received through inhalation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of 2-chloronaphthalene received through inhalation was 1.55 x10^{-8} mg/kg-day.

Treated drinking water

2-Chloronaphthalene was listed as a contaminant found in drinking water for a survey of US cities including Pomona, Escondido, Lake Tahoe and Orange County, CA, Dallas, Washington, DC, Cincinnati, Philadelphia, Miami, New Orleans, Ottumwa, IA, and Seattle (Lucas, 1984). In a study of 11 water utilities in the Ohio River Valley, 2-chloronaphthalene was detected in 4 of 150 raw water extracts and 30 of 120 finished drinking water extracts, suggesting that 2-chloronaphthalene is formed as a product of chlorination during water treatment (Ohio River Valley Water Sanitation Commission, 1980).

A Canadian laboratory study has shown that chloronaphthalenes may be formed from naphthalenes (an observed aquatic pollutant) under conditions similar to those used to disinfect drinking water and wastewater. This observation has led to speculation that treatment and the release in cooling water discharges and to drinking water supplies may be an ongoing source of chloronaphthalenes in the environment, despite the manufacture of chloronaphthalenes being discontinued in the 1970s. (Health and Welfare Canada, 1982). Current 2-chloronaphthalene concentrations in treated drinking water could not be located and an MCL does not exist for 2-chloronaphthalene.

Oceanic/marine levels

No information could be located concerning 2-chloronaphthalene concentrations in ocean waters, or bioconcentration factors in deep water ocean fish.

Soil and Sediments

On-site soil concentrations of 2-chloronaphthalene collected from a New Jersey landfill in 1987 averaged 3185 µg/kg, with a maximum of 12,000 µg/kg (USEPA,1988). The Florida Department of Environmental Protection has established a residential soil clean-up target level for 2-chloronaphthalene of 5000 mg/kg in accordance with Chapter 62-777, F.A.C (FDEP, 2005). The soil cleanup target concentration of 5000 mg/kg was used for RSC calculation under that assumption that it represents a highly conservative estimate of potential soil contamination levels. It represents a level above which the state would initiate cleanup protocols. Furthermore, it represents a high-end, as opposed to a central tendency, exposure level for the general population.

A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of 2-chloronaphthalene received through soil ingestion was 3.57 x10^{-3} mg/kg-day.

A 1992-1995 study to assess the occurrence of semi-volatile organic compounds in streambed sediments from 20 major river basins across the United States did not detect 2-chloronaphthalene at the 516 sites sampled (Lopes and Furlong, 2001). A survey of EPA's STORET database found that 340 sampling stations reported unspecified isomers of chloronaphthalene as present in sediments, of which 0.3% contained detectable levels of the chemical with a median concentration of less than 500 µg/kg by dry weight (Staples *et al*., 1985). Water and suspended solids samples were collected during June and August 1988 at four stations along the Rainy River on the Canada-Minnesota border and from two pulp and paper mill final effluents and were analyzed for a variety of organic contaminates. 2-Chloronaphthalene was detected in the suspended solids from one of the pulp and paper mill's final effluent at 18.0 and 21.0 ng/g in June and August, respectively. 2-Chloronaphthalene was not detected at the other five sites; the detection limit was 10.0 ng/g (Merriman *et al*., 1991).

Diet (other than fresh or estuarine fish)

Information and data concerning the concentrations of 2-chloronaphthalene detected in different food types are scarce. A number of incidental exposure reports associated with ingestion of polychlorinated naphthalenes (PCNs) exist, but are more representative of acute-type exposure scenarios and not what would necessarily represent exposure through chronic dietary intake. Incidents of consumption of contaminated rice oil occurred in Taiwan and China, with multiple contaminants identified, including PCNs, PCBs, PCDFs, PCQs, and PCDDs. (Kuratsune, 1989; Haglund *et al.,* 1995). PCNs were also reported in blood and adipose tissue specimens from the same events (Ryan and Masuda, 1994). Those effected experienced general systemic symptoms and severe chloracne. As reported by Falandysz (2003), Domingo *et al.* (2003), conducted a dietary intake study to determine the concentrations of polychloronaphthalenes in certain foods consumed by individuals in Catalonia, Spain. **Table 1** below includes the mean polychloronaphthalene concentrations for each food category, the intake rate for each associated food group obtained from EPA's 2011 exposure factors handbook, and the calculated dose received through ingestion of each food group.

Table 1. Exposure to polychloronaphthalenes through food-based dietary intake

Food Category	**Average Concentration (pg/g)**	**Intake Rate (g/kg-day)**	**Dose received through Exposure (mg/kg-day)**
Fruits	0.71	1.6	1.136 x10^{-9}
Vegetables	6.3	2.9	1.83 x10^{-8}
Meats	18	2.0	3.6 x10^{-8}
Dairy	59.37	6.6	3.92 x10^{-7}
Grains	71	2.6	1.85x 10^{-7}

Fats	450	1.2	5.4×10^{-7}

*Average food concentrations obtained from: Falandysz, J. (2003). Chloronaphthalenes as Food-Chain Contaminants: A Review. *Food Additives and Contaminants*, 20 (11): 995–1014. These concentrations are likely to represent a conservative assessment of chloronaphthalene concentrations in foods due to the fact that Domingo et al.'s (2003) analysis focused on polychloronaphthalenes, which possess a higher degree of chlorination, thus having a greater potential to accumulate in foods.

Ambient Exposure Sources

A survey of EPA's STORET database found 863 sampling stations that reported chloronaphthalenes (unspecified isomers) present in ambient waters, of which 1.4% contained detectable levels of the chemical with a median concentration of less than 10 µg/l. (Staples *et al.*, 1985). 2-Chloronaphthalene was detected at <2 µg/l in the Potomac River at Quantico, Virginia, in spring 1986 (Hall *et al.,* 1987). In September of 2005, the United States Environmental Protection Agency and the Mississippi Department of Environmental Quality conducted a water quality analysis of Bangs Lake, Bayou Casotte, the Pascagoula and West Pascagoula River systems, the Back Bay of Biloxi, St. Louis Bay, and the Pearl River to determine the effects of Hurricanes Katrina and Rita (USEPA, 2005B). Concentrations of 2-chloronaphthalene were below detection in both water and sediment sample analyses and the values reported represented the minimum limits of quantitation which are 10 ppb for water and 330 ppb for soils/sediments (USEPA, 2005B).

Levels of 2-chloronaphthalene were evaluated in oysters (*Crassostrea virginica*) and clams (*Rangia cuneata*) from Lake Pontchartrain, Louisiana. 2-Choronaphthalene levels were 34 µg/kg wet weight in oysters, and 140 and 970 g/kg wet weight in clams (IPCS, 2001B). 2-Chloronaphthalene was detected in multiple fish species in the Lake Michigan watershed, in White Lake and multiple river systems (Camanzo *et al*., 1987). 2-Chloronaphthalene was also detected in fish collected from multiple Great Lake harbors and tributary mouths (DeVault, 1985). According to the IPCS (2001B), chloronaphthalenes can be absorbed through the skin, lung, and gut, and tend to deposit in fat depots. These characteristics in combination with 2-chloronaphthalene's high BCF have the potential to positively impact the ability of chloronaphthalenes to bioaccumulate in fish species, especially those with a high lipid content.

RSC Calculation

The RfD for 2-chloronaphthalene for chronic oral exposure is 0.08 mg/kg-day (USEPA, 2013C). The inhalation of ambient air is expected to be a minimal to negligible source of exposure, based on studies in the United States that have shown that after the use of 2-chloronaphthalene was discontinued the compound was not detected in the air (Hunt *et al.,* 1982 and Foster *et al*., 1991, see above). If 2-chloronaphthalene is formed as a by-product during chlorination, as a few studies suggest, then drinking water could be a significant exposure route. The exposure of the general population to soils at solid waste sites, and suspended sediments in pulp and paper effluent streams, where 2-chloronaphthalene has been detected, is unknown. The exposure estimates described above were used to estimate a total non-ambient exposure dose of 3.57×10^{-3} mg/kg-day as summarized in **Table 2.**

Table 2. Estimated average daily 2-chloronaphthalene exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg-day)
Inhalation of air	1.55×10^{-8}
Soil ingestion	3.57×10^{-3}
Treated drinking water ingestion	No information available
Diet: Fruits	1.14×10^{-9}
Diet: Vegetables	1.83×10^{-8}
Diet: Meats	3.6×10^{-8}
Diet: Dairy	3.92×10^{-7}
Diet: Fats	5.4×10^{-7}
Diet: Grains	1.85×10^{-7}
Estimated total daily dose	3.57×10^{-3}

The total non-surface water exposure dose accounts for 4.5% of the 2-chloronaphthalene RfD of 0.08 mg/kg-day (USEPA, 2013C). Therefore, surface water sources can be allotted the remainder of the allowable exposure dose, resulting in a chemical-specific RSC of 0.955, or 95.5%. The chemical-specific RSC calculated for 2-chloronaphthalene is likely very conservative, as exposure estimates for soil and food do not account for the United States and Europe ceasing manufacture of Halowax in the late 1970s and due to the fact that FDEP's Chapter 62-777, F.A.C target soil clean up value was used to calculate the estimated exposure received through soil ingestion. Despite the conservative nature of the exposure estimate, it does not represent a full assessment of all potential exposure routes because it does not include treated drinking water exposures. Given the lack of information on this potential exposure route, FDEP recommends that a more conservative RSC value of 0.8 (*i.e.*, EPA ceiling) be used. Using this value assumes that treated drinking water exposures could potentially be as high as 5.35×10^{-3} mg/kg-day or at levels 1.5 times greater than exposures from all other exposures combined.

Toluene

Background

Toluene (CASRN108-88-3) exists as a clear liquid absent of any distinguishable color. Under circumstances where toluene exists at higher concentrations, this substance can be identified through a distinct smell distinguishable at air concentrations of 8 ppm and taste in water at concentrations ranging from 0.04 to 1.0 ppm (ATSDR, 2000). Toluene is produced in the process of making gasoline and other fuels from crude oil, in making coke from coal, and as a by-product in the manufacture of styrene (ATSDR, 2000). This substance is utilized in a wide variety of commercial products such as paints, paint thinners, fingernail polishes, lacquers, adhesive, rubbers, glues, solvents, and has been promoted as a safer alternative to the use of benzene (Fishbein, 1988). Individuals can be exposed to toluene through ingestion of foods or drinking water, inhalation of volatilized toluene from gasoline, consumer products, or dermal adsorption. However, according to

the ATSDR (1993), dermal exposure usually only causes skin irritation. When contact with the solvent is unusually extensive and prolonged, some systemic absorption can occur (ATSDR, 1993). The primary pathway of exposure to toluene is through inhalation. Toluene is a significantly volatile lipid-soluble substance that is also subject to microbial degradation in soils. Atmospheric degradation of toluene occurs through reactions with atomic oxygen, peroxy or hydroxyl radicals and ozone (WHO, 2004). Due to these characteristics, which occur in multiple types of environmental media (air, soil, water), the tendency for toluene to build up in the environment is minimal (ATSDR, 2000).

Exposure Source Determinations

Manufacturing and release

Toluene is a substance common to the manufacturing of many products and is released to the environment through anthropogenic activities. The largest source of toluene release occurs during the production, transport, and use of gasoline (OEHHA, 1999B). EPA's Chemical Data Access Tool (CDAT) reported that 3 producers in the United States have a national production volume of 2,467,872,276 lbs toluene/yr and have past production volumes of 1,202,631,333 lbs toluene/yr, 1,385,662,048 lbs toluene/yr, and 272,410,000 lbs toluene/yr (USEPA, 2013F).

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[11] of toluene in 2011 accounted for 28,006,459.09 pounds with the majority of release/disposal occurring through point source air emissions and fugitive air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[12] in 2011 accounted for 1,354,258.87 pounds of toluene with the majority of disposal/release occurring through RCRA Subtitle C landfill-based disposal and waste brokers (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for toluene in 2011 was 29,360,717.96 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 25,421,711.03 pounds of toluene with the majority of disposal/release

[11] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[12] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

occurring through point source air emissions and fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 1,305,250.74 pounds toluene with the majority of disposal/release occurring through "other off-site management", RCRA Subtitle C landfill-based disposal and waste brokers (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for toluene in 2012 was 26,726,961.77 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

According to Fishbein (1988), low levels of toluene, generally ranging from 1-5 µg/L, have been found in a number of American surface, tap, and drinking waters, although levels up to 12 µg/L have been reported in the drinking water and tap water of New Orleans, Louisiana. Literature and data pertaining to mean toluene concentrations typically found in treated drinking water are scarce. Therefore, to calculate the RSC for the drinking water ingestion route the Maximum Contaminant level (MCL), which defines the threshold above which water is not suitable for drinking, of 1000 µg/L was utilized because it represents a very conservative estimate of exposure. A standard water intake rate of 2.0 L/day and a standard body weight of 70 kg were also utilized in this calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of toluene received through drinking water ingestion was 0.029 mg/kg-day.

Groundwater

Toluene in groundwater exists as an artifact of improper/uncontained waste disposal, chemical spills, or leaks originating from apparatuses such as underground gasoline storage tanks. According to the WHO (2004) point source contamination of groundwater can cause toluene concentrations to spike with previously reported concentrations ranging from 0.2–1.1 mg/L. In approximately 1% of all groundwater-derived public drinking-water systems in the USA, toluene levels are above 0.5 µg/L (WHO, 2004). In 2009, the United States Environmental Protection Agency released their *Contaminant Occurrence Support Document for Category 1 Contaminants for the Second Six-Year Review of National Primary Drinking Water Regulations.* This support document contains and analyzes the national drinking water occurrence estimates for category 1 contaminants, toluene included, from the National Water Quality Assessment Program from 1992-2001. For groundwater, 4,545 samples were collected from 4,061 sites of which 13.1% of the samples detected toluene representing 13.9% of the sites sampled (USEPA, 2009B). Analysis of this data resulted in a median toluene concentration of 0.0356 µg/L, a 95th percentile concentration of 0.8845 µg/L, and a 99th percentile concentration of 12 µg/L (USEPA, 2009B).

Air

Toluene is a significantly volatile substance, thus ambient air exposures are of particular concern. This substance is estimated to have an atmospheric half-life of approximately 13 hours (ATSDR, 2000). Automobile emissions are the primary source of toluene in ambient air (ATSDR, 2000).

However, given the extensive presence of toluene in consumer and household products, indoor air possesses higher toluene concentrations than ambient outdoor air. For California in 1996, the mean statewide concentration for airborne toluene was measured as 2.26 ppb (OEHHA, 1999B). According to the United States Environmental Protection Agency's National Air Toxics Assessment (USEPA, 2005A), the 2005 report revealed that the total air concentration of toluene for the state of Florida was 2.63 $\mu g/m^3$. The United States Environmental Protection Agency reports that levels of toluene measured in rural, urban, and indoor air average 1.3, 10.8, and 31.5 micrograms per cubic meter ($\mu g/m^3$), respectively (USEPA, 2012C). For the purposes of RSC calculation, an outdoor air concentration of 10.8 $\mu g/m^3$ and an indoor air concentration of 31.5 $\mu g/m^3$ were utilized, based on the USEPA (2012C) values. An outdoor inhalation rate of 3.122 m^3/day, an indoor inhalation rate of 12.878 m^3/day, and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of toluene received through indoor inhalation was 5.80 x 10^{-3} mg/kg-day and the resultant estimated average daily dose of toluene received through outdoor inhalation was 4.82 x 10^{-4} mg/kg-day.

Oceanic/ marine levels

Information on typical concentrations of toluene detected in oceanic environments could not be located.

Soil

The tendency for toluene to exist in the adsorbed state within soils is dependent upon soil pH (IPCS, 1985). According to the WHO (2004), the extent to which toluene is biodegraded in soil ranges from 63% to 86% after 20 days. Information regarding typical toluene concentrations in soils could not be located. According to the ATSDR (2000), in the absence of continuous releases from a waste site, it is expected that toluene would not persist for long periods in soil, due to its volatility, susceptibility to biodegradation, and water solubility. Therefore, under typical exposure scenarios, exposure through soil ingestion is estimated to be negligible.

Diet (other than fresh or estuarine fish)

Residual concentrations of toluene are detected in a wide variety of food types. The United States Food and Drug Administration conducted an analysis of pesticide residuals in specific food types through their Total Diet Study program. The information summarized in this analysis pertains to Total Diet Study market baskets 1991-3 through 2003-4 collected between September 1991 and October 2003 (USFDA, 2006). FDEP analyzed each specific food type for reported toluene concentrations. Each food type was then separated into a distinct category: fruits, vegetables, meats, dairy, grain, fish (marine), and fats. Foods not included from the analysis were considered to be composite foods (*e.g.*, Quarter-pound hamburger on bun; Frozen dinner of Salisbury steak with gravy, potatoes, and vegetables; beef chow mein, from Chinese carry-out) covered by each previously delineated category. Toluene concentrations for each food category were then averaged and standard intake rates (USEPA, 2011A) were then utilized to calculate doses from exposure to each food group. **Table 1** provides the results of these calculations.

Table 1. Estimated exposure to toluene through food-based dietary intake.

Food Category	Average Concentration (ppm)	Intake Rate (g/kg-day)	Dose received through Exposure (mg/kg-day)
Fruits	0.00204	1.6	3.27×10^{-6}
Vegetables	0.00587	2.9	1.70×10^{-5}
Meats	0.0179	2.0	3.59×10^{-5}
Dairy	0.0215	6.6	1.42×10^{-4}
Fish (marine)	0.0267	0.22	5.80×10^{-6}
Grains	0.006272	2.6	1.63×10^{-5}
Fats	0.0155	1.2	1.85×10^{-5}

Exposures for potentially highly exposed individuals

Certain individuals may be exposed to higher concentrations of toluene than received by the general public. Occupations that require individuals to work with gasoline, paints, lacquers, or solvents may be exposed to higher concentrations of toluene on a daily basis due to the composition of these substances and the inherent nature of toluene to volatilize. Individuals who smoke cigarettes expose themselves to higher concentrations of toluene than found in ambient air. Smoking may contribute 1,000 µg/day or more of toluene to an individual's daily exposure (ATSDR, 2000). The dangerous and abusive habit of sniffing glues may increase an individual's exposure to toluene. Moreover, proximity to hazardous waste sites may also increase exposures to toluene.

Ambient Exposure Sources

Toluene exposures can also occur through ambient sources. According to the WHO (2004), toluene concentrations of 1 mg/kg have been reported in fish. Toluene is often taken up by aquatic organisms, but metabolism by aquatic biota often limits tissue accumulation of toluene (ATSDR, 2000). Bioaccumulation of toluene is ultimately dependent on the metabolic mechanisms and lipid content of the organism due to the fact that toluene is lipid-soluble. The National Water Quality Assessment Program data analysis shows that for surface water 1,394 samples were collected at 182 sites of which 69.4% of samples detected toluene associating 60.4% of sites sampled with positive detections (USEPA, 2009B). This analysis also reported a median surface water toluene concentration of 0.06 µg/L, 95th percentile concentration of 0.42 µg/L, and a 99th percentile concentration of 1.289 µg/L (USEPA, 2009B).

RSC calculation

The estimated doses received through daily exposure to toluene were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 2** below.

Table 2. . Estimated average daily toluene exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg-day)
Indoor air inhalation	5.80×10^{-3}
Outdoor air inhalation	4.82×10^{-4}
Treated Drinking Water ingestion	Negligible
Soil ingestion	0.029
Diet: Fruits	3.27×10^{-6}
Diet: Vegetables	1.70×10^{-5}
Diet: Meats	3.59×10^{-5}
Diet: Dairy	1.42×10^{-4}
Diet: Fish	5.80×10^{-6}
Diet: Grains	1.63×10^{-5}
Diet: Fats	1.85×10^{-5}
Estimated total daily dose	0.0355

The reference dose for toluene is 0.08 mg/kg-day (USEPA, 2013C). The estimated total non-ambient exposure of 0.0355 mg/kg-day represents 44.4% of the RfD. The remaining 55.6% is available for allocation to surface water exposures through routes such as estuarine fish consumption. Thus, a chemical specific RSC of 0.55 is suggested to be protective of human health and representative of toluene exposures received through ambient sources.

Polycyclic Aromatic Hydrocarbons: Acenaphthene, Anthracene, Fluoranthene, Fluorene, and Pyrene

Background

Polycyclic aromatic hydrocarbons (PAHs) constitute a large class of approximately 100 compounds. The U.S. EPA regulates 17 of these compounds and considers 5 to be primarily non-carcinogenic. PAHs are typically formed during incomplete combustion or pyrolysis of organic matter (*e.g.*, coal, oil, gas, wood, garbage, tobacco, charbroiled meat) and generally occur as complex mixtures, not as single compounds. As pure chemicals, PAHs generally exist as colorless, white, or pale yellow-green solids. They can have a faint, pleasant odor. A few PAHs are used in medicines and to make dyes, plastics, and pesticides. Others are contained in asphalt used in road construction. They can also be found in substances such as crude oil, coal, coal tar pitch, creosote, and roofing tar and are found throughout the environment in the air, water, and soil. They can occur in the air, either attached to dust particles or as solids in soil or sediment. At ambient temperatures, PAHs are solids. The general characteristics common to this class of compounds are high melting- and boiling-points, low vapor pressure, and very low water solubility, which tends to decrease with increasing molecular mass. PAHs are soluble in many organic solvents and are highly lipophilic.

Anthropogenic activities, such as combustion of fossil fuels, wood, and solid wastes, are the main inputs of PAHs to the environment (Baek *et al*., 1991). The annual emissions of PAHs have been estimated to be 8,600 tons in the USA and 14,100 ton in Europe (Kabziński, *et al*., 2002). Natural sources of PAHs, such as volcanic eruptions, forest fires, diagenesis of organic matter, and biochemical synthesis, are minor contributors of PAHs to the environment (Wilcke, 2000 and 2007). Among the anthropogenic sources, the petrogenic sources of PAHs include unburned petroleum and its products (gasoline, kerosene, diesel, and lubricating oil), whereas pyrogenic sources include high-temperature combustion products such as incomplete combustion of organic materials (combustion of fossil fuel, vehicular engine combustion, smelting, waste incinerators). The main anthropogenic sources of PAHs are power plants and house heating (51%). Incinerating plants and outdoor combustion are responsible for 28% emission to the atmosphere, industry (aluminum and steel foundries and gas engineering) for 20%, and (car) transportation is responsible for 0.9% of emissions (Skupinska *et al.*, 2004). Zang and Tao (2009) reported that similar to other developed countries, consumer product use (including personal care products, household products, automotive aftermarket products, adhesives and sealants, FIFRA-regulated products, and coatings, 35.1%) and traffic oil (23%) combustion were the major PAH emission sources in the United States, followed by waste incineration (9.5%), biofuel combustion (9.1%) and petroleum refining (8.7%).

Since PAHs have low vapor pressure and high octanol/air partition coefficients (log K_{ow} ~3 to 6), they tend to sorb strongly onto the soil mass and persist for a longer period of time (Wilcke, 2000). PAH concentrations in water tend to be extremely low (<100 ng/L) and instead accumulate in sediments and aquatic organisms (Skupinska *et al.,* 2004). For instance, Wild and Jones (1995) reported that 90% of the PAHs are strongly fixed and hence stored in the soils.

The greatest sources of exposure to PAHs for most Americans is through active or passive inhalation of the compounds in tobacco smoke, wood smoke, and contaminated air, and ingestion of these compounds in foodstuffs. Smoking one pack of cigarettes a day has been estimated to result in exposure to carcinogenic PAHs of up to 5 µg/day (Menzie *et al*., 1992). These compounds are in the exhaust from automobiles, coal, coal tar, and at hazardous waste sites. Exposure to other PAHs can occur by eating foods grown in contaminated soil or by eating meat or other food that is grilled. Contribution of motor vehicles to global PAH emissions is less than biomass burning and wildfires (Zhang and Tao, 2009). However, motor vehicle emissions occur mostly in urban areas where population densities are much higher. Consequently, relative contribution of PAHs from motor vehicles to human exposure risk is much greater than its contribution to total emissions.

Exposure Source Determinations

Manufacturing and release

Manufacturing and environmental release information/data for the individual polycyclic aromatic hydrocarbons under analysis could not be located utilizing the USEPA's Toxic Release Inventory (TRI) explorer tool.

Non-ambient Exposure Sources

Air

PAHs occur in the atmosphere in both the particle phase and the vapor phase. Three-ring PAH compounds are found in the atmosphere primarily in the gaseous phase, whereas, five- and six-ring PAHs are found mainly in the particle phase; four-ring PAH compounds are found in both phases. To fully characterize atmospheric PAH levels, both particle- and vapor-phase samples must be collected. Many early monitoring studies used filter sampling methods, which provided information on particle-phase PAH concentrations only and did not account for losses of some of the lower molecular weight PAHs by volatilization. As a result, the early use of particulate samples may have resulted in an underestimation of total PAH concentrations. More recent monitoring studies often use sampling methods that collect both particle- and vapor-phase PAHs that prevent or minimize volatilization losses, thus providing more reliable characterization of total atmospheric PAH concentrations (ATSDR, 1995D).

Deposition of PAH compounds directly to Tampa Bay was studied by Poor (2002) and Poor *et al*., (2004). In the 2002 study, measurements were made from March to October 2001. The average concentration for the total PAH in the ambient air was 14 ng/m^3. Dry deposition of gas and particles was estimated to be about 2 µg/m^2-day, and wet deposition of gas and particles was estimated to be about 0.1 µg/m^2-day, assuming no flux of PAHs from the water to the air. A comparison of these rates with others reported in the literature indicated that the rates in Tampa Bay are in the range of deposition rates at both rural and urban sites in the eastern coastal U.S. (Poor, 2002). The 2004 study used a sampling method, which improved capture of gas and particle-phase PAH compounds with lower molecular weights. Based on sampling between May and August 2002, the concentrations of total PAHs were between 80 and 190 ng/m^3, and dry deposition flux of gas and particles was estimated to be 11.5 µg/m^2-day, assuming no flux of PAH from the water to the air. The 2004 study reported both gas-phase and particle-phase ambient air concentrations for individual PAHs. The mean values are reproduced in **Table 1**. Additionally, FDEP calculated daily exposures for the general population using the total concentration for each PAH. The air concentration values listed in **Table 1** are comparable, although higher if summed, to the total PAH ambient air concentration of 10.9 ng/m^3 provided by Santodonato *et al*., (1981). The differences may be related to the fact that the value reported by Santodonato was based on the sum of annual geometric means, rather than arithmetic means, only included 14 individual PAHs, and did not include acenaphthene or fluorene.

Table 1. Average daily ambient air concentrations of gas- and particle-phase PAHs measure by Poor *et al*., (2004) at the Grandy Bridge in Tampa, FL.

PAH	Mean gas-phase (ng/m^3)	Mean particle-phase (ng/m^3)	Total gas- and particle-phase (ng/m^3)	Intake[1] (mg/kg-day)
Acenaphthene	4.07	0.20	4.27	$1.90 \cdot 10^{-7}$
Anthracene	0.50	0.00	0.50	$2.23 \cdot 10^{-8}$
Fluoranthene	4.91	0.99	5.90	$2.63 \cdot 10^{-7}$
Fluorene	6.15	0.27	6.42	$2.86 \cdot 10^{-7}$
Pyrene	1.74	0.61	2.35	$1.05 \cdot 10^{-7}$

1. Calculated from total gas- and particle-phase concentration and an assumption of a daily outdoor inhalation volume of 3.122 m^3.

Sheldon *et al*., (1993) summarized a 1992 study of indoor air pollution in 280 California homes. Housing units were selected to represent homes in specific source categories based on both the presence and expected use of several combustion sources, including fireplaces, woodstoves, gas heating, and tobacco smokers (**Table 2**). Li *et al*., (2005) conducted a survey of indoor PAHs in residential air of ten Chicago area non-smoker homes. Mean indoor air concentrations were interpolated from a figure presented in Li *et al*., (2005) and are summarized in **Table 3**. They also reported that the mean total indoor air PAH concentration, excluding naphthalene (15 compounds), was 36 ng/m^3. Following naphthalene, anthracene was found to have the second highest indoor air concentration. FDEP calculated daily indoor inhalation exposures for the general population using the total concentration provided by both Sheldon *et al.,* (1993) and Li *et al*., (2005) for each PAH. The highest daily intake rate for each compound was used in subsequent RSC calculations.

Table 2. Average indoor PAH air concentrations (ng/m^3) by combustion source category from Sheldon *et al*., (1993).

Compound	Smoking (ng/m^3)	Smoking/ Fireplace (ng/m^3)	Fireplace (ng/m^3)	Woodstove (ng/m^3)	Woodstove/ Gas Heat (ng/m^3)	Gas Heat (ng/m^3)	No Source (ng/m^3)	Max (ng/m^3)	Intake[1] (mg/kg-day)
Anthracene	2.3	2.2	2.9	3.2	2.4	2.2	2.7	3.2	$5.89 \cdot 10^{-7}$
Fluoranthene	5.3	4.5	5.3	7	4.6	4.7	5.2	7	$1.29 \cdot 10^{-6}$
Pyrene	5.3	4.9	5.1	6.5	4.2	4.5	5	6.5	$1.20 \cdot 10^{-6}$

1. Calculated from total gas- and particle-phase concentration and an assumption of a daily indoor inhalation volume of 12.878 m^3.

Table 3. Average indoor air PAH concentrations by combustion source category from Li *et al*., (2005).

Compound	Mean Indoor Air Concentration (ng/m^3)	Intake[1] (mg/kg-day)
Acenaphthene	3.8	$6.99 \cdot 10^{-7}$
Fluorene	4.6	$8.46 \cdot 10^{-7}$
Anthracene	9.7	$1.78 \cdot 10^{-6}$
Fluoranthene	2.2	$4.05 \cdot 10^{-7}$
Pyrene	1.2	$2.21 \cdot 10^{-7}$
Total PAH	36	$6.62 \cdot 10^{-6}$

1. Calculated from total gas- and particle-phase concentration and an assumption of a daily indoor inhalation volume of 12.878 m^3.

Diet (other than fresh or estuarine fish)

Food is the main source of non-occupational exposure to PAHs for humans. Unprocessed foods do not typically contain high levels of PAHs. In areas isolated from urban or industrial activities, the levels of total PAHs found in unprocessed foods (0.01-1 µg/kg) reflect the background

contamination, which originates from long distance airborne transportation of contaminated particles and natural emissions from volcanoes and forest fires. In the vicinity of industrial areas or along highways, the contamination of vegetation can be ten-fold higher than in rural areas (Larsson and Sahlberg, 1982).

Processing of food (*e.g*., cooking, drying, smoking) and cooking of foods at high temperatures (*e.g*., grilling, roasting, frying) are major sources generating PAHs (Guillen *et al.*, 1997; Phillips, 1999). Although not precisely known, it is likely that there are several mechanisms associated with the formation of PAHs. These mechanisms could include examples such as melted fat that undergoes pyrolysis when dripping onto the heat and pyrolysis of the meat due to the high temperature. (Lijinsky and Shubik, 1965A, 1965B). Individual PAH concentrations as high as 200 µg/kg have been detected in smoked fish and meat. PAH concentrations of 130 µg/kg have been reported in barbecued meats, whereas the average background values are usually in the range of 0.01-1 µg/kg in uncooked foods. A comparison of PAH levels in duck breast steaks, undergoing various processing and cooking treatments for 0.5 hours to 1.5 hours, showed that charcoal-grilled samples without skin contained the highest amount of total PAHs (320 µg/kg), followed by charcoal grilling with skin (300 µg/kg), smoking (210 µg/kg), roasting (130 µg/kg), steaming (8.6 µg/kg) and liquid smoke flavoring (0.3 µg/kg).

Gomaa *et al*., (1993) reported the results of a study to screen smoked foods, including turkey, pork, chicken, beef, fish products, and commercial liquid smoke flavorings, for carcinogenic and non-carcinogenic PAHs. All smoked meat products and liquid smoke seasonings were purchased from local supermarkets in Michigan. Total PAH concentrations in smoked red meat products ranged from 2.6 µg/kg in cooked ham to 29.8 µg/kg in grilled pork chops, while those in smoked poultry products ranged from 2.8 µg/kg in smoked turkey breast to 22.4 µg/kg in barbecued chicken wings. Total PAH concentrations in smoked fish products ranged from 9.3 µg/kg in smoked shrimp to 86.6 µg/kg in smoked salmon. Total PAH concentrations in liquid smoke flavorings and seasonings ranged from 6.3 to 43.7 µg/kg. Smoked meat products processed with natural wood smoke had higher total PAH and total carcinogenic PAH concentrations than those processed with liquid smoke flavorings. Contamination of vegetable oils with PAHs usually occurs during technological processes like direct fire drying, where combustion products may come into contact with the oil seeds or oil (Speer *et al.*, 1990; EC, 2002). It is clear that PAH concentrations in food range considerably depending on the preparation. Likewise, exposure to individuals within the population likely also varies considerably, perhaps over an order of magnitude, depending on an individual's diet and food preferences. The final RSC calculations included a consideration of this order of magnitude variation in exposure related to diet; that is, dietary exposure was increased by a factor of 10 as an added level of conservatism.

The EC (2002) compiled comparative intake data for individual PAHs. Intake data was gathered from five total diet studies conducted in the United Kingdom (two studies: Dennis *et al.*, 1983; COT, 2002), Italy (Turrio-Baldassarri *et al.*, 1996), the Netherlands (De Vos *et al.*, 1990) and Austria (Pfannhauser, 1991). Benzo[*a*]pyrene intakes were also available for Sweden (Beckman Sundh *et al.*, 1998), Germany (IPCS, 1998) and the USA (Butler *et al.*, 1993; Kazerouni *et al.*, 2001). EC

(2002) provided mean daily intake of individual PAHs via food consumption (**Table 4**). The estimates presented in **Table 4** are based on European rather than U.S. or Floridian populations. However, EC (2002) provides a comparison between U.S. benzo[*a*]pyrene food intake rates to European countries. Mean benzo[*a*]pyrene intake in the U.S. (mean=0.14 µg/day) was estimated to be similar yet slightly lower than the European Union (0.05-0.29 µg/day), suggesting that European intake rates could be used as representative estimates for the U.S. population and may in fact be slightly conservative. Santodonato *et al*., (1981) estimated that total PAH (including carcinogenic PAHs) concentrations in food typically range from 0.1 to 10 ppb (ng/g). The total PAH exposure estimates are an order of magnitude greater than individual PAHs, and can be used as conservative estimates of food-related exposures for PAHs lacking individual estimates (*i.e*., acenaphthene and fluorene).

Table 4. Estimated daily exposure intake of individual non-carcinogenic PAHs via dietary (food) intake. Daily intake was estimated using the upper end of the exposure range.

PAH	Daily per Capita Exposure (ng/person-day)	Daily Intake (mg/kg-day)
Acenaphthene	N/A	0.00029[1]
Anthracene	<30-640	0.000009[2]
Fluoranthene	600-1660	0.000024[2]
Fluorene	N/A	0.00029[1]
Pyrene	600-1090	0.000016[2]
Total PAH[1]	2030-20,300	0.00029[1]

1. Estimated from Santodonato *et al*., (1981) based on average body weight of 70 kg and total daily food consumption of 29 g/kg-day.
2. Estimated daily average adult intakes from EC (2002).

Soil

PAHs are ubiquitous in soil. Because anthropogenic combustion processes are a major source of PAHs in soils, soil concentrations have tended to increase over the last 100-150 years, especially in urban areas (Jones *et al*., 1989A, 1989B). Background concentrations for rural, agricultural, and urban soils (from the United States and other countries) are given in **Table 5**. In general, concentrations ranked as follows: urban > agricultural > rural. Evidence of the global distribution of PAHs was given by Thomas (1986) who detected benzo[g,h,i]perylene and fluoranthene at concentrations above 150 µg/kg in arctic soils. Soil samples collected from remote wooded areas of Wyoming contained total PAH concentrations of up to 210 µg/kg.

Table 5. Background soil concentrations of polycyclic aromatic hydrocarbons (PAHs). Table recreated after ATSDR (1995).

Compound	Rural Soil (µg/kg)	Agricultural Soil (µg/kg)	Urban Soil (µg/kg)
Acenaphthene	1.7	6	

Anthracene		11-13	
Fluoranthene	0.3-40	120-210	200-166,000
Fluorene	9.7		
Pyrene	1-19.7	99-150	145-147,000

Several researchers have observed a greater amount of PAHs in urban soils as these areas are more exposed than rural areas to the PAHs produced by both stationary (power plants, industries, and residential heating) and diffused sources (traffic emissions, and road byproducts such as wearing of tires and asphalt constituents). For instance, Maisto *et al*., (2006) reported that total PAHs were 2-20 times greater in the urban areas of Naples, Italy, than park soils that were 12 km away. Similarly, Baek *et al.* (1991) reported that the urban soils near the highways were highly contaminated. In New Orleans, Wang *et al.* (2008) observed the higher amounts of PAHs in soils close to the roads (7,189 µg/kg) than in open spaces that were 10 m away from the roads (2,404 µg/kg). Similar results were shown by Wilcke (2000), who reported that PAH levels declined exponentially with increase in distance from the roads due to the reduced vehicular emissions. In Northern Germany, Krauss and Wilcke (2003) found that the PAHs in gardens and industrial soils (> 10 µg/kg) were eightfold greater than the park soils (1.9 µg/kg) while the lowest amounts were observed in agricultural soils (0.64 µg/kg).

Chahal *et al*., (2010) determined PAH contamination levels in urban residential soils in Pinellas County, FL. They reported mean soil levels for all non-carcinogenic PAHs under consideration, except acenaphthene (**Table 6**). Wang *et al*., (2008) reported PAHs from two major US cities, New Orleans and Detroit. Sampling sites included house foundations, open spaces, and soils bordering residential (light to moderate traffic) and busy (heavy traffic) streets. Results from soils in the vicinity of busy streets are not reproduced here under the reasoning that although the contamination level may be higher than other areas, the general population exposure to soils from these areas is negligible given that few people will spend much time, particularly engaging in activities that might lead to soil ingestion, in these areas due to safety concerns. The soil concentrations from New Orleans and Detroit tend to be higher than Pinellas County, FL; however, the estimated daily doses are within an order of magnitude for all parameters. Both studies represent conservative estimates of general population exposure to PAHs through incidental soil consumption. They are conservative in that both studies represent urban areas with extensive and long-term motor vehicle traffic as well as industrial development. Less developed and less highly traveled areas of the state are likely to have lower contamination levels. Use of the daily intake values listed in **Tables 6** and **7** are therefore conservative for the general population while also being protective and representative of potential exposures for urban and suburban populations. The Florida-specific exposures from Chahal *et al*., (2010) were used to calculate RSC values for anthracene, fluoranthene, flourene and pyrene, while Wang et al., (2008) was used for acenaphthene.

Table 6. Mean soil concentrations for individual PAHs in Pinellas County, FL as reported by Chahal *et al*., (2010). Daily intakes were calculated from the mean soil concentrations.

PAH	Mean Soil (µg/kg)	Daily Intake (mg/kg-day)
Acenaphthene	N/A	
Anthracene	110	$7.86 \cdot 10^{-8}$
Fluoranthene	133	$9.50 \cdot 10^{-8}$
Fluorene	33	$2.36 \cdot 10^{-8}$
Pyrene	297	$2.12 \cdot 10^{-7}$

Table 7. Mean soil concentrations for individual PAHs in New Orleans and Detroit as reported by Wang *et al*., (2008). Daily intakes were calculated from the overall mean soil concentrations.

Soil Location	Units	Acenaphthene	Anthracene	Fluoranthene	Fluorene	Pyrene
Open Space: New Orleans	(µg/kg)	11.5	36.5	365	13.7	378
Open Space: Detroit	(µg/kg)	15.6	24.1	447	3.4	408
Foundation: New Orleans	(µg/kg)	23.6	76.5	949	27.9	751
Foundation: Detroit:	(µg/kg)	7.2	29.8	451	5.5	366
Street Side: New Orleans	(µg/kg)	26.5	63.1	936	20.6	793
Street Side: Detroit	(µg/kg)	14.5	49.3	926	5.4	740
Range	(µg/kg)	7.2-26.5	365-949	3.4-27.9	24.1-76.5	366-793
Mean	(µg/kg)	16.5	679	12.8	46.6	573
Daily Intake	(mg/kg-day)	$1.18 \cdot 10^{-8}$	$4.85 \cdot 10^{-7}$	$9.14 \cdot 10^{-9}$	$3.33 \cdot 10^{-8}$	$4.09 \cdot 10^{-7}$

Treated drinking water

Santodonato *et al*., (1981) summarized work by Basu and Saxena (1978) and reported that the average total PAH level in U.S. drinking water is 13.5 ng/L. Santodonato noted that EPA also conducted the Nation Organic Monitoring Survey to determine the frequency of occurrence and the levels of PAHs in U.S. drinking water supplies. Of the 110 water samples analyzed, none showed any PAHs other than fluoranthene. Seventeen out of 110 samples analyzed showed positive fluoranthene values with an average of 20 ng/L concentration. Kabziński *et al.*, (2002) provided estimates of individual PAH concentrations in drinking water from several Polish Cites (**Table 8**). Although the level of fluoranthene in Polish drinking water is very similar to the EPA calculated average for the US, the individual PAH values from the Polish study are all greater than the total PAH estimate provided by Santodonato *et al*., (1981) for the United States. The drinking water concentrations provided by Kabziński *et al.,* (2002) were used to calculate estimated daily intake values for each PAH (**Table 8**). Alternatively, a total PAH intake rate of 0.000386 µg/kg-day can be estimated from the drinking water concentration provided in Santodonato *et al*., (1981).

Table 8. Mean drinking water PAH concentrations (ng/L) reported by Kabziński *et al.*, (2002). The average concentrations were calculated from the reported means and an estimate of parameter specific intake was calculated from this average.

PAH	Łódź-Chojny Area (ng/L)	Łódź-Stoki Area (ng/L)	Tomaszów Mazowiecki Area (ng/L)	Average (ng/L)	Intake[1] (mg/kg-day)
Acenaphthene	38	25	39	34	$9.71 \cdot 10^{-7}$
Anthracene	69	56	71	65	$1.87 \cdot 10^{-6}$
Fluoranthene	22	19	20	20	$5.81 \cdot 10^{-7}$
Fluorene	175	133	141	150	$4.28 \cdot 10^{-6}$
Pyrene	22	19	20	20	$5.81 \cdot 10^{-7}$

1. Calculated based on average concentration, 70 kg body weight, and daily drinking water intake of 2.0 L (USEPA 1997; NRC, 1977).

Ambient Exposure Sources

Staples *et al*., (1985) summarized priority pollutant concentration in the United States using results from the STORET Database. They reported median ambient surface water concentrations of <10.0 µg/L with a four percent detection rate for all five non-carcinogenic PAHs. National sample sizes ranged from 776 for anthracene to 904 for pyrene. Ambient surface water data were queried from the IWR Run 47 database and the range of measured concentrations over the ten-year period from 2002-2011 were summarized (**Table 9**). None of the five PAHs under consideration were detected in Florida surface waters based on average detection limits of approximately 2.0 µg/L.

Table 9. Summary of PAH concentrations in Florida surface waters. Data were taken from the IWR Run 47 database for the period from 2002 to 2010.

PAH	Number of Samples	Minimum Detection Limit (µg/L)	Average Detection Limit (µg/L)
Acenaphthene	314	0.04	2.26
Anthracene	353	0.03	2.09
Fluoranthene	351	0.022	2.14
Fluorene	282	0.04	1.25
Pyrene	352	0.021	2.15

Staples *et al*., (1985) reported biota tissue priority pollutant concentrations using STORET data. They reported median tissue concentrations of <2.5 mg/kg for each acenaphthene, anthracene, fluoranthene, fluorene, and pyrene with no detections. In 2011, FDEP undertook a study to determine if the water quality of Clam Bayou located in Pinellas County, has degraded over time. The Department assessed the biological, chemical, sediment, and physical characteristics of Clam Bayou. A total of 63 chemicals, including PAHs, were analyzed for in 36 fish tissue samples (12 individual fish samples of three different species from Clam Bayou fish representing the different

trophic levels and feeding strategies). Average fish tissue concentrations for the non-carcinogenic PAH concentrations are summarized in **Table 10**.

Table 10. Chemical analysis of fish tissue samples collected from Clam Bayou on September 29, 2011.

PAH	*Archosargus probatocephalus* (Sheepshead) (mg/Kg)	*Centropomus undecimalis* (Common snook) (mg/Kg)	*Mugil cephalus* (Striped mullet) (mg/Kg)
Acenaphthene	0.00063	0.00055	0.00193
Anthracene	0.00054	0.00050	0.00067
Fluoranthene	0.00200	0.00089	0.00475
Fluorene	0.00145	0.00150	0.00255
Naphthalene	0.00137	0.00196	0.00183
Pyrene	0.00176	0.00066	0.00182

RSC Calculation

The exposure estimates described above were used to estimate a total non-surface water exposure dose as summarized below in **Table 11**. In all cases, the total non-ambient exposure to non-carcinogenic PAHs accounted for less than 1 percent of the applicable RfD. Additionally, because there is likely to be significant variability in PAH exposures, particularly related to diet, FDEP investigated the effects of increasing the total dietary exposure by an order of magnitude (factor of 10). Even under this scenario non-ambient exposures would account for only 0.03 to 7.3% of the applicable RfDs (**Table 12**). FDEP used the available exposure data to support protective RSC values for all five PAHs in excess of 92% with clear margin of safety, including individuals who consume greater quantities of smoked or grilled foods. Therefore, FDEP will use RSC values listed in **Table 12** for the non-carcinogenic PAHs.

Table 11. Tabulation of non-surface water exposures (mg/kg-day) to non-carcinogenic PAHs for the general population.

Exposure	Acenaphthene	Anthracene	Fluoranthene	Fluorene	Pyrene
Outdoor air inhalation	$1.90 \cdot 10^{-7}$	$2.23 \cdot 10^{-8}$	$2.63 \cdot 10^{-7}$	$2.86 \cdot 10^{-7}$	$1.05 \cdot 10^{-7}$
Indoor air inhalation	$6.99 \cdot 10^{-7}$	$1.78 \cdot 10^{-6}$	$1.29 \cdot 10^{-6}$	$8.46 \cdot 10^{-7}$	$1.20 \cdot 10^{-6}$
Soil ingestion	$1.18 \cdot 10^{-8}$	$7.86 \cdot 10^{-8}$	$9.50 \cdot 10^{-8}$	$2.36 \cdot 10^{-8}$	$2.12 \cdot 10^{-7}$
Treated drinking water ingestion	$9.71 \cdot 10^{-7}$	$1.87 \cdot 10^{-6}$	$5.81 \cdot 10^{-7}$	$4.28 \cdot 10^{-6}$	$5.81 \cdot 10^{-7}$
Diet	$2.90 \cdot 10^{-4}$	$9.00 \cdot 10^{-6}$	$2.40 \cdot 10^{-5}$	$2.90 \cdot 10^{-4}$	$1.60 \cdot 10^{-5}$
Estimated total daily dose	$\mathbf{2.92 \cdot 10^{-4}}$	$\mathbf{1.28 \cdot 10^{-5}}$	$\mathbf{2.62 \cdot 10^{-5}}$	$\mathbf{2.95 \cdot 10^{-4}}$	$\mathbf{1.81 \cdot 10^{-5}}$

Table 12. Summary of lower and upper range total non-surface water source exposure to five PAHs and selected RSC values. The lower range exposures were tabulated in **Table 11** above. The upper range estimates were calculated by increasing dietary (food) exposures by a factor 10. The selected RSCs were calculated from the upper end exposure estimate.

Parameter	Exposure Lower Estimate (mg/kg-day)	Exposure Upper Estimate (mg/kg-day)	Percent RfD	RSC
Acenaphthene	$2.92 \cdot 10^{-4}$	$2.90 \cdot 10^{-3}$	0.49-4.84%	0.95
Anthracene	$1.28 \cdot 10^{-5}$	$9.38 \cdot 10^{-5}$	0.004-0.03%	1.0
Fluoranthene	$2.62 \cdot 10^{-5}$	$2.42 \cdot 10^{-4}$	0.07-0.61%	0.99
Fluorene	$2.95 \cdot 10^{-4}$	$2.91 \cdot 10^{-3}$	0.74-7.26%	0.92
Pyrene	$1.81 \cdot 10^{-5}$	$1.62 \cdot 10^{-4}$	0.06-0.54%	0.99

Nitrobenzene

Background

Nitrobenzene (CASRN 98-95-3) is a synthetic colorless to pale yellow, oily liquid with an odor resembling that of bitter almonds or shoe polish. Ninety-five percent of nitrobenzene is used in the production of aniline, a major chemical intermediate that is used in the manufacture of polyurethanes. Nitrobenzene is also used as a solvent in petroleum refining, as a solvent in the manufacture of cellulose ethers and acetates, in the manufacture of dinitrobenzenes and dichloroanilines, and in the synthesis of other organic compounds, including acetaminophen. Nitrobenzene had some use, in the early 20th century, as a food additive (substitute for almond essence) as well as extensive use as a solvent in various proprietary products, including boot polish, inks and several disinfectants. Most (97% to 98%) of the nitrobenzene produced is retained in closed systems for use in synthesis of aniline and other substituted nitrobenzenes and anilines, thus limiting its release into air (ATSDR, 1990).

There was a significant increase in annual production of nitrobenzene between the 1950's and 1990's (ATSDR, 1990). The demand for nitrobenzene has increased steadily from 73,000 metric tons) in 1960 to 1,390,000 metric tons by 2007 (IARC, 1996; Bizzari and Kishi, 2007). In 1995, nitrobenzene ranked 49th in volume among chemicals produced in the United States (Kirschner, 1996). In 2009, there were 5 U.S. producers and 20 U.S. suppliers of nitrobenzene (SRI, 2009). Imports and exports of nitrobenzene are reported to be negligible (ATSDR, 1990; HSDB, No.104).

Nitrobenzene has a vapor pressure of 0.245 mm Hg at 25° C indicating that the compound exists solely as a vapor in the atmosphere. Vapor-phase nitrobenzene will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals. The half-life for this reaction in air is estimated to be 115 days. In the atmosphere, nitrobenzene should degrade primarily by photolysis (38% degradation in 5 hr). If released to soil**,** nitrobenzene is expected to have very high to moderate mobility based upon K_{oc} values of 30.6 to 370. Volatilization from moist soil surfaces is expected to be an important fate process based upon a Henry's Law constant of 2.4×10^{-5} atm-

m^3/mole. Nitrobenzene is expected to biodegrade under both aerobic and anaerobic conditions in both soil and water. Nitrobenzene had a half-life of 56 days in an aerobic soil column**.** Nitrobenzene was rapidly biodegraded after a lag phase of 70 to 85 days in an aerobic aquifer test done with groundwater and sediment from 8 locations over a 149 day incubation period. Nitrobenzene is not expected to adsorb to suspended solids and sediment in water based upon a K_{oc} of 89 measured in river sediment. Nitrobenzene may be degraded in water by photolysis (a half-life of 133 days), by reaction with hydrated electrons in eutrophic lakes (a half-life of 22 days), or by reaction with sunlight and nitrate (a measured half-life of 11 hours). Volatilization from water surfaces is expected to be an important fate process based upon this compound's Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 44 hours and 17 days, respectively. Bioconcentration values ranging from 1.47 to 28.32 suggest that bioconcentration in aquatic organisms is low (HSDB, No.104).

The general population can be exposed to nitrobenzene in air and possibly drinking-water. There is also potential exposure from consumer products, but accurate information is lacking. Based on air studies and on estimates of releases during manufacture, only populations in the vicinity of manufacturing activities and petroleum refining plants are likely to have any significant exposure to nitrobenzene (ATSDR, 1990). However, people living in and around abandoned hazardous waste sites may also have the potential for higher exposure, due to possible groundwater and soil contamination and uptake of nitrobenzene by plants. Exposure is mitigated by environmental degradation, including photolysis and microbial biodegradation. Nitrobenzene is poorly bioaccumulated and not biomagnified through the food chain (ATSDR, 1990).

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[13] of nitrobenzene in 2011 accounted for 303,286.83 pounds with the majority of release/disposal occurring through underground injection to Class I wells and point source air emissions (TRI2011, 2013A). Total reported off-site disposal or

[13] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[14] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

other releases[14] in 2011 accounted for 756.57 pounds of nitrobenzene with the majority of disposal/release occurring through RCRA Subtitle C landfill-based disposal and other landfills (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for nitrobenzene in 2011 was 304,043.40 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 240,302.25 pounds of nitrobenzene with the majority of disposal/release occurring through underground injection to Class I wells and point source air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 227 pounds nitrobenzene with the majority of disposal/release occurring through "other land disposal" and RCRA Subtitle C landfill-based disposal (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for nitrobenzene in 2012 was 240,529.25 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Air

Direct release of nitrobenzene to air during its manufacture is minimized by the passage of contaminated air through activated charcoal (USEPA, 1983), and its subsequent use in closed systems as an intermediate similarly limits direct exposure during industrial processing. Much of the information on nitrobenzene levels in air is derived from a series of reports from New Jersey, USA, in which ambient air in urban, rural, and waste disposal areas was monitored extensively. In the initial study by Bozzelli *et al*., (1980), nitrobenzene was not detected above the level of 0.05 μg/m^3 in about 260 samples collected in 1979. In 1978, nitrobenzene levels averaged 2.0 μg/m^3 in industrial areas and 0.1 μg/m^3 and 0.46 μg/m^3 in two residential areas; in 1982, levels in residential areas were approximately 1.5 μg/m^3 or less, whereas levels in industrial areas were 46 μg/m^3 or more (Bozzelli and Kebbekus, 1982). Nitrobenzene was not detected in most samples.

Little information is available for other areas of the United States. Pellizzari (1978) found only one positive value of 107 ng/m^3 at a plant site in Louisiana. The USEPA (1985) summarized data showing that less than 25% of US air samples were positive, with a median concentration of about 0.05 μg/m^3. Mean levels measured in urban areas are generally low (<1 μg/m^3), whereas slightly higher levels (mean 2.0 μg/m^3) have been measured in industrial areas.

Harkov *et al.,* (1983, 1984) carried out a comparison of the concentrations of nitrobenzene at several urban sites in New Jersey, USA. In the summer, the geometric mean levels detected at three sites were 0.35, 0.35 and 0.5 μg/m^3, with 80–90% of the samples being above the detection limit of 0.25 μg/m^3. In contrast to this, nitrobenzene was detected in only 6–14% of the samples taken in the winter. Hunt *et al*., (1986), using the data collected by Harkov *et al.* (1984), calculated the arithmetic means for the three sites as 0.96, 1.56 and 2.1 μg/m^3 in the summer and 0.050, 0.050

[14]

and 0.10 µg/m^3 in the winter. In another study (Lioy *et al.,* 1983), nitrobenzene was not detected during the winter.

Table 1 summaries air-based nitrobenzene concentrations from a number of studies. The overall mean of U.S. studies is 0.742 µg/m^3, which translates to a daily inhalation exposure of 0.17 µg/kg-day. The inhalation exposure was calculated based on 70 kg body weight and 16 m^3/day inhalation volume (USEPA, 1997; USEPA, 2011A). This inhalation exposure estimate represents an extremely conservative value for Florida because it is biased towards highly industrialized areas in New Jersey.

Table 1. Measured levels of nitrobenzene in air from various literature sources.

Location (samples)	Mean level (µg/m^3)	Reference
Camden, USA, July–August 1981 (24-h average)	0.96 (max. 10.0)	Hunt *et al.*, 1986
Camden, USA, January–February 1982 (24-h average)	0.050 (max. 0.75)	Hunt *et al.*, 1986
Elizabeth, USA, July–August 1981 (24-h average)	1.56 (max. 24.1)	Hunt *et al.*, 1986
Elizabeth, USA, January–February 1982 (24-h average)	0.050 (max. 0.35)	Hunt *et al.*, 1986
Newark, USA, July–August 1981 (24-h average)	2.1 (max. 37.5)	Hunt *et al.*, 1986
Newark, USA, July–August 1982 (24-h average)	0.10 (max. 1.26)	Hunt *et al.*, 1986
Six sites in New Jersey, USA (sampled every 6 days for 1–2 years)	<0.050	Bozzelli & Kebbekus, 1982
Industrial site, New Jersey, USA (241 samples)	2.0	Bozzelli & Kebbekus, 1982
Residential site, New Jersey, USA (49 samples)	0.10	Bozzelli & Kebbekus, 1982
Residential site, New Jersey, USA (40 samples)	0.45	Bozzelli & Kebbekus, 1982
Japan	0.14 (range 0.0022–0.16)	Environment Agency Japan, 1992

Emissions and modeled nitrobenzene concentrations were queried from the EPA National-Scale Air Toxics Assessment (NATA; USEPA, 2013D). NATA is EPA's ongoing comprehensive evaluation of air toxics in the United States. EPA developed NATA as a state-of-the-science screening tool for state/local/tribal agencies to prioritize pollutants, emission sources, and locations of interest for further study in order to gain a better understanding of risks. NATA assessments do not incorporate refined information about emission sources, but rather, use general information about sources to develop estimates of risks which are more likely to overestimate impacts than underestimate them. The resulting risk estimates are purposefully more likely to be overestimates of health impacts than underestimates, and thus they are health protective.

FDEP downloaded the most recent NATA results (USEPA, 2005A). Data for all Florida and New Jersey counties were queried from the database http://www.epa.gov/ttn/atw/nata2005/tables.html. New Jersey was queried because the majority of nitrobenzene studies have been conducted in the state and there was thus an interest in evaluating the degree by which New Jersey-based estimates would overestimate conditions in Florida. **Table 2** summarizes the statewide total (combined point and nonpoint sources) and maximum by county nitrobenzene air concentration estimate for each state. Average daily exposures were additionally calculated for both Florida and New Jersey (**Table 2**). These estimates suggest that average and maximum nitrobenzene in the air are 17 and 132 times, respectively, greater in New Jersey than in Florida (**Table 2**).

Table 2. Average and maximum air concentrations across all Florida and New Jersey Counties based on data from NATA (2005). Average concentrations are based on the statewide estimates while the maxima represent the highest county value reported in NATA (2005). Average daily intakes were calculated based on average concentrations, a daily inhalation volume of 16 m^3/day, and a body weight of 70 kg (USEPA, 2011A; USEPA, 1997).

State	Average Air Concentration (µg/m^3)	Maximum Air Concentration (µg/m^3)	Average Intake (µg/kg-day)
FL	2.10×10^{-6}	5.32×10^{-6}	4.79×10^{-7}
NJ	3.56×10^{-5}	7.04×10^{-4}	1.37×10^{-5}

Groundwater

Nitrobenzene is infrequently reported in groundwater. It was detected in groundwater at 3 of 862 hazardous waste sites in the USA at a geometric mean concentration of 1400 µg/L, according to the Contract Laboratory Program Statistical Database (CLPSD, 1988). Nitrobenzene was not detected (<1.13 µg/L) in groundwater at an explosives manufacturing site in the U.S., although the aquifer at the site was known to be contaminated with explosives residues (Dennis *et al*., 1990; Wujcik *et al*., 1992). Nitrobenzene was also detected at a level of 210–250 µg/L in groundwater from Gibbstown, New Jersey (Rosen *et al.,* 1992). The IPCS (2003B) reported that nitrobenzene, measured at a concentration of 4.2 mg/L, was detected in groundwater at a coal gasification site in the U.S.

Treated drinking water

Kopfler *et al*. (1977) listed nitrobenzene as one of the chemicals found in finished tap water in the USA, but did not report its concentrations or locations. Nitrobenzene was detected in 1 of 14 samples of treated water in the United Kingdom. The positive sample was water derived from an upland reservoir (Fielding *et al.,* 1981B). In a survey of 30 Canadian potable water treatment facilities, nitrobenzene was not detected in either raw or treated water (detection limit 5 µg/L) (Otson *et al.,* 1982). According to the BUA (1994) as cited in IPCS (2003B), the nitrobenzene content in potable water was 0.1 µg/L (mean), with maximum values of 0.7 µg/L in 50 samples taken from the river Lek at Hagestein, Netherlands, in 1986. FDEP used the 0.1 µg/L value from BUA (1994) as a conservative estimate of tap water concentration. Estimated daily exposure via

ingestion of tap water (0.00286 µg/kg-day) was calculated based on the concentration, a standard body weight of 70 kg, and daily water intake of 2.0 liters (USEPA, 1997; NRC, 1977).

Soil

As a potential nitrobenzene exposure source, soil is less important than air or groundwater. Nelson & Hites (1980) reported a nitrobenzene concentration of 8 mg/kg in the soil of a former dye manufacturing site along the bank of the industrially polluted Buffalo River in New York, USA, but failed to detect nitrobenzene in river sediments. Exposure via soil intake is unlikely to be a source for the general population given that only low concentrations have been detected at former manufacturing sites at which the general population has extremely limited access. Additionally, given the extremely low atmospheric concentrations ($1.05x10^{-6}$ µg/m^3), atmospheric deposition is expected to be negligible outside of manufacturing areas; thus, soils outside of manufacturing sites are highly unlikely to be contaminated and the estimated exposure can be assumed to be negligible.

Other sources

Nitrobenzene has not been found in other environmental media. Data on nitrobenzene occurrence in foods were not located in the available literature. No monitoring of plant tissues has been reported, even though uptake of nitrobenzene by plants has been observed (McFarlane *et al.* 1987A, 1987B). General population exposure via their diets is expected to negligible for the same reasons as soils.

Oceanic/marine levels

Information on nitrobenzene levels in marine fish and shellfish was not found in the literature. Likewise, data and information on nitrobenzene levels in marine waters is also limited. Weigal *et al*., (2005) quantified pesticides and industrial chemicals in the North Sea. They reported nitrobenzene concentrations ranging from 0.26 to 4.4 ng/L. The highest concentrations (2.5-4.4 ng/L) were in areas influenced by the river Elbe. Concentrations within the central regions of the North Seas were typically around 0.7 ng/L. A conservative estimate of nitrobenzene concentrations in marine fish tissue can be calculated using the EPA bioconcentration factor of 2.89 multiplied by a conservative ocean water concentration of 4.4 ng/L, resulting in an estimated ocean fish tissue concentration of 12.72 ng/kg. A marine fish consumption rate of 0.22 g/kg-day was conservatively assumed to estimate daily exposure via marine fish ingestion of $2.8x10^{-6}$ mg/kg-day. This estimated exposure is highly conservative for the general population and assumes that all fish consumed originate from the most highly contaminated waters.

Ambient Exposure Sources

Staples *et al*., (1985) summarized priority pollutant concentrations in the United States using the STORET Database. A median nitrobenzene concentration of <10 µg/L based on 836 samples with a 0.04% detection rate was reported. Ambient surface water data were queried from the IWR Run 47 database and the range of measured concentrations over the ten-year period from 2002-2011 were summarized (n=303). There were no detections over the period of record based on detection limits ranging from 0.19 to 10 µg/L (mean=2.5 µg/L). The IPCS (2003B) reviewed available data

and reports and concluded that surface water concentrations were generally low ranging from 0.1 to 1 µg/L.

Nitrobenzene is infrequently reported in fish tissue. It has not been detected as a bioaccumulated material in fish samples based on a review of STORET data (Staples *et al.* 1985). Surveys of nitrobenzene in fish were carried out in Japan in 1991. Nitrobenzene was detected in 4 of 147 fish samples at a level of 11–26 µg/kg (detection limit 8.7 µg/kg) (Environment Agency Japan, 1992).

RSC Calculation

Exposure of the general population to nitrobenzene is limited to air and possibly drinking water at extremely low levels. Air levels can be high in the vicinity of manufacturing or production facilities (especially petroleum refining, leather finishing and some chemical manufacturers). Based on air studies and on estimates of releases during manufacture, only populations in the vicinity of manufacturing activities (*i.e.*, producers and industrial consumers of nitrobenzene for subsequent synthesis) and petroleum refining plants are likely to have any significant exposure to nitrobenzene.

Table 3 provides a tabulation of all quantified non-ambient exposure routes for the general population to nitrobenzene. The total non-surface water exposure dose accounts for 0.28 to 8.8 percent of the nitrobenzene RfD of 0.002 mg/kg-day. Therefore, surface water sources potentially can be allotted the remainder of the allowable exposure dose, resulting in a chemical-specific RSC of 0.912 to 0.997. However, information on several potential exposure routes is lacking. These exposures are most likely negligible given the facts that nitrobenzene is typically contained within closed industrial processes and the extremely low (and infrequently detected) concentrations in air and water. Thus, it is highly unlikely that food or soil is contaminated at levels that would significantly alter the RSC. FDEP selected the lower (0.91) RSC estimate for use in development of human health criteria. The lower (more conservative) value was selected because not all potential exposure routes could be quantified, although it is highly likely that these are negligible and the selected RSC is therefore highly conservative. The RSC value is largely based on the range of exposure estimates developed for inhalation of air, which were developed from data collected in highly industrialized areas.

Table 3. Estimated average daily nitrobenzene exposure received through non-ambient sources by the general population.

Exposure Route (Non-Surface Water Sources)	**Estimated Exposure (mg/kg-day)**
Inhalation of Air	1.70E $x10^{-4}$ - 4.79 $x10^{-10}$
Soil ingestion	Negligible
Treated drinking water ingestion	2.86 $x10^{-6}$
Diet	Negligible
Diet: Marine fish	2.8 $x10^{-6}$
Estimated total daily dose	**1.75 x 10^{-4} - 5.66 x 10^{-6}**

Butylbenzyl Phthalate (BBP)

Background

Butylbenzyl phthalate (BBP) (CASRN 85-68-7) is a phthalate ester used as a plasticizer to add flexibility to plastics. BBP is more specifically used in PVC-based flooring products (foam flooring tiles), polyvinyl acetate emulsion adhesives, cellulose resins, sealants, foams, adhesives, inks, car care products, and cosmetics (HSDB, No. 2107). It has been found in traffic cones, food conveyor belts, and artificial leather (NTP-CERHR, 2003).

According to the U.S. Department of Health and Human Service's National Toxicology Program (NTP-CERHR, 2003), the most likely route of exposure to the general population is from food that has come into contact with BBP during processing. Although, Clark *et al.,* (2011) notes accidental ingestion of dust and inhalation of air also contribute to total exposure. The given information suggests that toddlers have the greatest exposure risk. In terms of environmental fate, photooxidation is the most important process for the breakdown of BBP in the atmosphere and biodegradation under aerobic conditions represents the most important degradation pathway for surface waters, soils, and sediments (IPCS, 1999).

Exposure Source Determinations

Manufacturing and release

According to the U.S. National Library of Medicine's Toxic Release Inventory, there have not been any releases of BBP to the environment since 1993 (TRI2011, 2013A). However, according to EPA's Chemical Data Access Tool (USEPA, 2013F), there are 4 producers of BBP in the U.S., each manufacturing between 50,000,000 and 100,000,000 lbs. of BBP/year.

Non-ambient Sources

Diet (other than fresh or estuarine fish)

Out of 100 foods tested, the International Program on Chemical Safety (IPCS) found BBP in four foods: yogurt, cheddar cheese, butter, and crackers (IPCS, 1999). They estimate a total daily intake of 2 µg/kg with the threat to infants and children possibly being 3 times higher (NTP-CERHR, 2003). The UK's Ministry of Agriculture, Fisheries, and Food (MAFF), measured BBP in formula from below detect to 0.24 µg/g. However, infants in the U.S. are likely exposed to lower levels according to a 1996 study in the U.S. measuring BBP in formula (NTP-CERHR, 2003). BBP is approved by the FDA as an indirect food additive in the manufacturing and processing of food provided that the butyl benzyl phthalate contains no more than 1 percent by weight of dibenzyl phthalate (USFDA, 2013). A 2000-2001 study from the USEPA (2011B) looked at total exposure to BBP in preschool aged children from Ohio and North Carolina. They estimated daily intake to be 10 µg/kg-day based on median estimates from individual sources (based on Ohio children; NC exposure was reported as lower). Sources included in the study were indoor and outdoor air, soil, dust, drinking water, food, and dermal absorption. This estimate was used to conservatively represent exposure through food.

Drinking Water and Soil

Estimated total exposure calculated by the IPCS considered exposures from drinking water and soil intake are negligible (NTP-CERHR, 2003).

Air

Due to butyl benzyl phthalate's low vapor pressure, exposure from air is expected to be minimal (NTP-CERHR, 2003). In a survey of 125 California homes, the median air levels of BBP ranged from 0.034-0.035 ng/m^3 (IPCS, 1999). At 65 of the California homes, samples of outdoor air were also collected. The median outdoor air concentration was below the detected limit of 0.051 ng/m^3, while the 90th percentile values ranged from 5.3 to 6.7 ng/m^3. For the purposes of RSC calculation, the 90th percentile exposure range (5.3 to 6.7 ng/m^3) was utilized. A conservative daily (90th percentile) exposure range from 1.21 x10^{-6} to 1.53x10^{-6} mg/kg-day was calculated based on a standard daily inhalation rate of 16 m^3 and a standard body weight of 70 kg (USEPA, 2011A; USEPA, 1997).

Dermal contact

Studies in rats have shown that absorption through dermal contact is possible but fairly slow at 27% in 7 days (Elsisi, 1989). Also, it has been demonstrated that the permeability of human skin to other ester phthalates (DBP and DEHP) is much lower than that of rat skin (Scott, 1987).

Other Media

BBP is reportedly not in children's toys (NTP-CERHR, 2003). One study measuring BBP in 17 toys showed that only one contained BBP at 0.02% by weight (Rastogi, 1998). BBP is not approved by the FDA for use in medical devices (NTP-CERHR, 2003).

Consumer and personal care products

Several million tons of phthalates are used each year in the production of soft polyvinyl chloride and other plastics that are used in many consumer and personal care products (*e.g.*, makeup, deodorant, perfume, nail polish). Due to the fact that phthalates are not chemically-bound constituents of the products they are incorporated within, potential release to ambient air can occur. Although BBP is not among the most commonly used phthalate plasticizers, it still may be used in many products that consumers may come in contact with. Thus, exposure through consumer product contact could possibly be an additional significant exposure route.

Measured concentrations from indoor air would take into consideration some of the exposure from consumer products encountered by the general population. However, these indoor air estimates do not consider short-term and likely greater exposures associated with the direct use of consumer products. Additionally, indoor air estimates do not account for dermal or oral exposures, particularly for at risk populations, such as children and women. Children, especially very young children may be at a greater risk of exposure due their behavioral patterns. They drink more fluids, have a larger skin surface in proportion to their body volume, they may consume more dairy products, they crawl on the floor/ground, put things in their mouths, and/or may eat inappropriate things (like dirt or paint chips) (ATSDR, 2001). Women, in general, may use more personal care products, such as makeup, perfume, or nail polish, than do men.

Wormuth *et al.* (2006) conducted an extensive analysis of exposure to eight phthalate esters, including BBP, for European populations. The analysis included exposures from inhalation of indoor air, outdoor air, and while using spray paints; dermal exposure from personal care products, gloves, and textiles; and oral exposure from food, dust, mouthing (young children) and ingestion of personal care products. They estimated daily exposures for seven age and gender groups (consumer groups): infants (0-12 months, 5.5 kg bw); toddlers (1-3 years, 13 kg bw); children (4-10 years, 27 kg bw); male adolescents (11-18 years, 57.5 kg bw); male adolescents (11-18 years, 57.5 kg bw); female adults (18-80 years, 60 kg bw); and, male adults (18-80 years, 70 kg bw). FDEP used the mean exposures for each consumer group as an additional line of evidence in evaluating the RSC for BBP. This additional line of evidence provided information on the protectiveness of the RSC calculated using the typical exposure routes (diet, inhalation, drinking water, and soil and dust ingestion), when additional potential exposure through consumer products is also considered.

Ambient Exposure Sources

Bioconcentration factors in bluegill sunfish (*Lepomis macrochirus)* were estimated by Carr *et al.,* (1997) to be 9.4 for the whole fish and only 1.7 for the fillet. These estimates were much lower than predicted based on previously published BCFs based on the whole fish (Carr *et al.,* 1997). In addition, BBP was detected in 3% of 1,220 of U.S. waters with a median of <10.0 µg/L using STORET data (Staples *et al.,* 1985).

RSC Calculation

Based on the information gathered by the IPCS (1999), they concluded that food is the only significant source of BBP. They estimated total exposure to be approximately 2 µg/kg-day. Clark *et al*., (2011) estimates exposure from food to make up 68-77% of the total exposure for adults, teens, children, and toddlers with the remaining exposure from ingestion of dust and inhalation of indoor air. For infants, ingestion of dust accounts for 94% of total exposure with the remainder from food. Wormuth *et al.,* (2006) found that in adults 60% of exposure was from food, while the remainder was from the inhalation of spray paint (and vice versa for teens). Clark *et al.,* (2011) agree that for children, food is the dominant exposure pathway. The Clark *et al.* study (2011) summarizes total exposures from both intake and primary metabolite studies, shown below.

Table 1. Summary of total estimated exposure studies (intake and biomarker) from Clark *et al.* (2011).

Study	Study Type	Geographical Area	Exposure Routes	Intake/Exposure (µg/kg-day)
Clark *et al.,* (2003)	Intake	Various	Diet, air, dust	0.49-1.5 (medians across age groups)

Study	Study Type	Geographical Area	Exposure Routes	Intake/Exposure (µg/kg-day)
Wormuth *et al.* (2006) + supplemental data	Intake	Europe	Oral, inhalation, and dermal	0.11-1.6 (intermediate estimates across age groups)
Wilson *et al.* (2003)	Intake	United States	Composite diet, dust, soil, inhalation of indoor and outdoor air	1.9 (mean; age 2-5 years only)
CDC (2005)(2001-2002 NHANES data)	Primary metabolite	United States	-	0.33-0.70 (geo means across age groups and genders)
Marsee *et al.* (2003) (pregnant women)	Primary metabolite	United States	-	0.50 (median)
Brock *et al.* (2002)	Primary metabolite	United States	-	1.5 (geo mean; age 11.8-16.5 months)
CDC (2003)(1999-2000 NHANES data)	Primary metabolite	United States	-	0.32-0.73 (geo means across age groups and genders)

As described above, Wormuth *et al.*, (2006) evaluated total BBP exposure in seven consumer groups. Their analysis included additional exposure from consumer and personal care products. They concluded that infants were the most highly exposed group followed by toddlers (**Table 2**). Dust was reported as the main source of exposure to BBP in infants and toddlers (>70%) followed by food (20%) and air (5%). Food was reported as the major source in children (73%) with indoor air accounting for 26% of exposure for this group. Spray paints were reported as major exposure routes in teenagers (>70%) and adults. Food accounted for 20 and 60 percent of exposures in teenagers and adults, respectively.

Table 2. Mean daily exposure to for butylbenzyl phthalate in seven consumer groups taken from Wormuth *et al*. (2006).

Consumer Group	Mean Total Daily Exposure (mg/kg-day)
Infant	0.00073
Toddlers	0.00031
Children	0.00004
Female Teen	0.00015
Male Teens	0.00019
Female adults	0.00028
Male Adults	0.00031

Table 3 provides the estimated average daily exposure of the general public to butyl benzyl phthalate. Even though all exposure routes were analyzed, dietary exposure through food-based consumption is the dominant exposure route. All other environmental media/sources of exposure had a minimal to negligible influence on the total calculated exposure.

Table 3. Estimated average daily butyl benzyl phthalate exposure received through non-ambient sources by the general population.

Exposure Route (Non-Surface Water Sources)	Estimated Exposure (mg/kg-day)
Inhalation of air	1.05×10^{-6} to 2.22×10^{-6}
Soil ingestion	Negligible
Treated drinking water ingestion	Negligible
Diet	0.010
Estimated total daily dose	**0.010**

The estimates of total exposure represents a very small fraction of the RfD (200 µg/kg-day) for butylbenzyl phthalate. Including diet, which is the most significant source, the highest exposure estimate (10 µg/kg-day; exposure to preschool children from USEPA, 2011B) makes up 5 percent of the RfD. The 5% value is highly likely to be a conservative estimate based on several considerations. First, extreme care must be taken with phthalate ester samples to avoid false high values. Clark *et al.* (2011) notes that the analysis of phthalate esters is plagued by contamination issues and requires rigorous sample handling and quality control to exclude phthalate ester contamination from sources inside and outside the analytical laboratory. Thus, care must be taken during analysis as not to overestimate exposure in the various sampled mediums due internal or external factors that have the potential to confound the outcomes of analysis. Secondly, BBP has not been released to the environment in the United States since 1993, although large amounts are still manufactured. Third, estimates from Wormuth *et al.,* (2006) showed much lower levels of exposure in all consumer groups, including infants and toddlers, even when additional exposures from consumer and personal care products were considered (**Table 2**). Furthermore, it is also expected to volatilize rapidly from water due to its Henry's Law constant estimation of 1.3×10^{-6}

atm- m^3/mole, thus minimizing exposures through water. The information supports a conservative RSC for butylbenzyl phthalate of 0.95.

Dimethyl phthalate (DMP)

Background

Dimethyl phthalate (DMP) (CASRN 131-11-3) is a phthalate ester used in manufacturing solid rocket propellant and consumer products such as insect repellants, lacquers, safety glasses, rubber coating agents, molding powders, pesticides, and plastics (Lewis, 2007). Acute exposure via inhalation in humans, results in irritation of the eyes, nose, and throat (HSDB, No. 1641; New Jersey DOH, 1986). DMP can be breathed in and may be absorbed through the skin. Data suggests that the general population may be exposed to dimethyl phthalate through inhalation of ambient air, ingestion of drinking water, and dermal contact with products containing DMP (HSDB, No. 1641). Its former use as an insect repellent resulted in its direct release to the environment (Lewis, 2007). DMP occurs in nature as a metabolite of *Gibberella fujikuroi* (O'Neil, 2006), which is a fungus that causes 'cotton boll rot' and is found in Florida.

DMP is a colorless oily liquid with a slightly sweet odor (New Jersey DOH, 1986). Its vapor pressure is 3.09×10^{-3} mm Hg at 25°C (Daubert, 1989), which indicates it can be found in both vapor and particulate phases in the atmosphere (Bidleman, 1988). Vapor phase DMP is degraded in the air by reaction with photochemically-produced hydroxyl radicals. It's half-life in the air is expected to be 28 days (HSDB, No. 1641). While the particulate phase of DMP is removed by wet or dry deposition, it is also subject to direct photolysis by sunlight since it contains chromophores that absorb at wavelengths greater than 290 nm (HSDB, No. 1641).

In soil, DMP is expected to have high to moderate mobility based on its log K_{oc} of 55-360 (Osipoff, 1981). It has a Henry's Law Constant of 2.0×10^{-7} atm-m^3/mole, which makes volatilization from moist soil surfaces unexpected (HSDB, No. 1641). Biodegradation half-lives in contaminated soil ranging from 15 to 123 days (Kincannon and Lin, 1985) suggest that biodegradation is dependent on prior exposure and subsequent acclimation (HSDB, No. 1641).

If released into water, dimethyl phthatlate is expected to adsorb to suspended solids and sediment based upon its mean Koc value of greater than 5.2 (Ritsema, 1989). A 50 percent biodegradation in 1 to 5 days with complete disappearance obtained in 2 to 13 days in sediment-water estuarine and freshwater sites suggest that biodegradation may be an important environmental fate process in water (Walker, 1984; HSDB, No. 1641). Volatilization from water surfaces is not expected to be an important fate process (Lyman, 1990) based upon this compound's estimated Henry's Law constant (HSDB, No. 1641).

Bioconcentration factors of 5.4 and 4.7 for sheepshead minnows (Wofford, 1981) and 57 in bluegill sunfish (Barrows, 1980) suggest bioconcentration in aquatic organisms is low to moderate (HSDB, No. 1641). Bioaccumlation in *Peneaus aztecus* (brown shrimp) were 3.1 and 6.3 (Giam, 1984). Aerobic degradation studies indicated primary degradation for the lower molecular weight phthalate esters (which include DMP) occurred rapidly, typically exceeding 90% degradation within a week (Staples *et al.,* 1997). Microorganisms isolated from soil are capable of utilizing dimethyl phthalate (Williams, 1983). Microorganisms from natural waters are also able to use DMP

(Taylor, 1981). Ritsema (1989) showed that DMP was completely degraded in 2 to 13 days in sediment-water systems obtained from 6 different estuarine and freshwater sites bordering the Gulf of Mexico.

Exposure Source Determinations

Manufacturing and release

There were no releases of DMP in 2011 to surface waters (TRI2011, 2013A). 482 pounds were released to the air in Florida in 2011. There is also a very large release to the atmosphere by Ruskin Co., in Geneva, Alabama, which is just over the Florida-Alabama state line (TRI2011, 2013A). They released 13,685 pounds in 2011, the largest amount by any facility nationwide.

At a national level, total reported on-site disposal or other releases[15] of dimethyl phthalate in 2011 accounted for 99,248.17 pounds with the majority of release/disposal occurring through point source air emissions and fugitive air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[16] in 2011 accounted for 6674.16 pounds of dimethyl phthalate with the majority of disposal/release occurring through " other landfills" and "other off-site management" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for dimethyl phthalate in 2011 was 105,922.34 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 88,558.74 pounds of dimethyl phthalate with the majority of disposal/release occurring through point source air emissions and fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 4,021.57 pounds dimethyl phthalate with the majority of disposal/release occurring through landfill-based disposal (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for dimethyl phthalate in 2012 was 92,580.31 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

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[15] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[16] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

DMP was detected in drinking water at 3 New Orleans plants ranging from 0.13 to 0.27 µg/L (Keith *et al.,* 1976). DMP has been detected in other sources in Philadelphia (Suffet, 1976), England (Fielding *et al.,* 1981A), Japan (Akiyama, 1980), and Cincinnati, OH (Lucas, 1984). Note that many of the concentrations mentioned above, were determined over 20 years ago. Clark *et al.,* (2011) provided an estimated mean concentration of 0.027 µg/L for drinking water. For the purposes of RSC calculation, the Clark *et al.* (2011) estimate of 0.027 µg/L was used to calculate exposure via drinking water for the general population. A standard drinking water intake rate of 2.0 L/day and a standard body weight of 70 kg were also used in the calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of DMP received through ingestion of drinking water was 7.71×10^{-7} mg/kg-day.

Groundwater

Little information could be located regarding dimethyl phthalate concentrations in groundwater. However, a DMP concentration was reported as detected in groundwater in Massachusetts at 0.10 µg/L (Bedient, 1983).

Air

DMP was not detected in 70 samples collected outside of office buildings in US cities in Kansas, Texas, New Jersey, Wisconsin, or Montana (Shields, 1996). In indoor air, DMP was detected in Wisconsin (0.43 to 0.60 µg/m^3) and New Jersey (1.54 to 1.74 µg/m^3) in 1987 (Shields, 1987). In 1988, it was detected in an office building also in Wisconsin, at concentrations ranging from 0.7 to 1.2 µg/m^3. Clark *et al.* (2011) reported a mean DMP indoor air concentration of 0.923 µg/m^3 and a mean DMP outdoor air concentration of 0.0033 µg/m^3. For the purposes of RSC calculation, the mean DMP values of 0.923 µg/m^3 for indoor air and 0.0033 µg/m^3 for outdoor air were utilized because they represent the most recent mean concentrations of DMP the general population would be exposed to through inhalation. An indoor inhalation rate of 12.878 m^3/day, an outdoor inhalation rate of 3.122 m^3/day, and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DMP received through inhalation of indoor air was 1.70×10^{-4} mg/kg-day and the resultant estimated average daily dose of DMP received through inhalation of outdoor air was 1.47×10^{-7} mg/kg-day.

Soil and dust

Due to the ubiquitous nature of phthalates in consumer products, these chemicals can become incorporated into soils and household dusts. Various DMP soil concentrations were located within literature. DMP was detected in 6 out of 10 soils in Canada. Results were not quantified, but the detection limit was 0.03 mg/kg dry weight (Webber, 1995). Clark *et al.* (2011) reported a mean ingested soil concentration of 0.0002 µg/g, Mcfall (1985) reported DMP soil concentrations of 0.002 and 0.0002 (µg/g) and Lopes and Furlong (2001) reported a DMP soil concentration of 0.12 (µg/g). For the purposes of RSC calculation, an average incorporating each of these concentrations was taken. Thus, a DMP soil concentration of 0.0306 µg/g was tabulated for RSC purposes. A soil ingestion rate of 20 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DMP received through soil ingestion was 8.74×10^{-9} mg/kg-day. Clark *et al.* (2011) reported a mean DMP ingested dust concentration

of 2.0 µg/g. For the purposes of RSC calculation, this concentration was utilized to represent DMP dust exposure. A dust ingestion rate of 30 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DMP received through dust ingestion was 8.57×10^{-7} mg/kg-day.

Diet (other than fresh or estuarine fish)

Dimethyl phthalate concentrations were measured for but not detected in 57 vodka and spirit bottles (Leibowitz, 1995). DMP was also measured for but not detected in corn grain, carrot, and cabbage samples collected at a coal refuse reclamation site in Illinois (Webber, 1994). In a study which tested coffee filters, it was detected in 1 of 10 filters at a concentration of 2.0 µg/g (Fricker, 1990). Clark *et al.* (2011) analyzed but did not detect DMP in a variety of foods, including water, cereals, dairy, eggs, fats and oils, fruit, grains, meats, nuts and beans, poultry, processed meats, vegetable products, and others. DMP was detected in fish and milk at 0.0012 µg/g and 0.7 µg/L, respectively. The concentration estimates associated with fish and milk originating from the Clark *et al.,* (2011) study were used as a line of evidence to calculate DMP exposure associated with dietary intake of these items.

Personal care and consumer products

Several million tons of phthalates are used each year in the production of soft polyvinyl chloride and other plastics that are used in many consumer and personal care products (e.g., makeup, deodorant, perfume, nail polish). Phthalates are not chemically bound to the products they are constituents of and are released continuously into the air. Although DMP is not among the most commonly used phthalate plasticizers, it still may be used in many products thus creating a pathway for potential exposure especially for women who often utilize personal care products more so than men and children who possess a lower threshold of exposure.

Wormuth *et al.* (2006) conducted an extensive analysis of exposure to eight phthalate esters, including DBP, for European populations. The analysis included exposures from inhalation of indoor air, outdoor air, and while using spray paints; dermal exposure from personal care products, gloves, and textiles; and, oral exposure from food, dust, mouthing (young children) and ingestion of personal care products. They estimated daily exposures for seven age and gender groups (consumer groups): infants (0-12 months, 5.5 kg bw); toddlers (1-3 years, 13 kg bw); children (4-10 years, 27 kg bw); male adolescents (11-18 years, 57.5 kg bw); male adolescents (11-18 years, 57.5 kg bw); female adults (18-80 years, 60 kg bw); and, male adults (18-80 years, 70 kg bw). Mean daily dimethyl phthalate exposures for these groups reported by Wormuth *et al.* (2006) are reported below in **Table 1**. FDEP used the mean exposures for each consumer group as an additional line of evidence in evaluating the RSC for DMP. This additional line of evidence provided information on the protectiveness of the RSC calculated using the typical exposure routes (diet, inhalation, drinking water, and soil and dust ingestion), when additional potential exposure through consumer products is also considered.

Table 1. Total Mean Daily Exposure to Dimethyl Phthalate in Seven Consumer Groups taken from Wormuth *et al*. (2006).

Consumer Group	Mean Total Daily Exposure (µg/kg-day)
Infant	$1.99 \cdot 10^{-3}$
Toddlers	$7.40 \cdot 10^{-4}$
Children	$5.10 \cdot 10^{-4}$
Female Teen	$2.20 \cdot 10^{-4}$
Male Teens	$2.50 \cdot 10^{-4}$
Female adults	$2.30 \cdot 10^{-4}$
Male Adults	$2.30 \cdot 10^{-4}$

Ambient Exposure Sources

DMP was detected in the Mississippi River at 0.002 and 0.005 µg/L (DeLeon, 1986). Using data in STORET, DMP was detected in 6% of samples at concentrations below 10 µg/L (Staples *et al*., 1985). Sediment samples from Lake Ponchartrain, LA contained 0.2 and 2.0 ng/g dry weight dimethyl phthalate (McFall, 1985). DMP was detected in 0.6% of 521 sites sampled in 20 major river basins across the United States from 1992-1995 with a maximum concentration of 120 µg/kg dry weight (Lopes and Furlong, 2001). DMP has been detected in oysters and clams from Lake Pontchartrain, LA at concentrations of 8.4 ng/g and 44 ng/g wet weight (McFall, 1985). DMP concentrations ranging from 0.58- 2.28 ng/g lipid were measured in a variety of marine organisms (invertebrates and fish) in 1999 from British Columbia (MacKintosh, 2004).

RSC Calculation

Considering the RfD for dimethyl phthalate is 10 mg/kg-day (USEPA, 1980D), the total documented exposure is extremely small and may be characterized as negligible. The most comprehensive and recent assessment of general population exposure to DMP was provided by Clark *et al.,* (2011). Their estimates were used to calculate a total non-ambient exposure. **Table 2** summarizes the concentrations, daily intake, and total exposure. The total non-surface water exposure dose accounts for less than 0.002% percent of the DMP RfD of 10 mg/kg-day. The total exposures calculated by FDEP are slightly higher, for the general population, than those reported by Wormuth *et al*. (2006) when consumer and personal care products are additionally considered. Infants are potentially exposed at a greater rate (approximately 10 times); however, almost 100% of this exposure was caused by indoor air rather than exposures regulated under the Clean Water Act (*i.e*., drinking water and fish consumption). Furthermore, total exposures for all consumer groups reported by Wormuth *et al.* (2006) account for the less than 0.02% of the RfD. FDEP concluded that although a total non-ambient dose could be quantified it is negligible or trivial in comparison to the RfD; therefore, FDEP recommends an RSC of 1.0 for DMP.

Table 2. Tabulation of non-surface water exposures to dimethyl phthalate for the general population. All exposures, with the exception of marine fish, were calculated based on a body weight of 70 kg. A body weight was not used for marine fish because the intake is provided on per kilogram basis.

Source	Mean concentration	Intake rate	Estimated Exposure (mg/kg-day)
Indoor air[1]	0.923 µg/m3	12.878 m^3/day	1.70×10^{-4}
Outdoor air[2]	0.0033 µg/m3	3.122 m^3/day	1.47×10^{-7}
Drinking water[3]	0.027 µg/L	2 L/day	7.71×10^{-7}
Soil[4]	0.0306 µg/g	20 mg/day	8.74×10^{-9}
Dust[5]	2.0 µg/g	30 mg/day	8.57×10^{-7}
Fish[6]	0.012 µg/g	0.22 g/kg-day	2.64×10^{-6}
Milk[7]	0.7 µg/L	0.226 L/day	2.26×10^{-6}
Total			1.76×10^{-4}

1. The concentration used for indoor air was taken from the mean given in Clark *et al.* (2011).
2. Little information on outdoor air concentrations could be found so the concentration from Clark *et al.* (2011) was used.
3. The drinking water concentration given in Clark *et al.* (2011) of 0.027 µg/L was lower than the estimates given on the HSDB of 0.13-0.27ug/L (1976). However, the estimate from Clark *et al.* (2011) was chosen to be utilized due to the fact that it is more recent.
4. Concentrations found in soil varied, the mean of four measured concentrations (from Clark *et al.*, 2011; McFall 1985; and, Lopes and Furlong, 2001) was used for calculations.
5. Clark *et al.* (2011).
6. Concentrations found in fish varied greatly. The mean of five concentrations (from McFall 1985, MacKintosh 2004, and the mean given in Clark *et al.* (2011) was used in calculations. Fish were included in this dietary exposure estimate due to the fact that they were assumed not to have come from Florida waters.
7. Milk intake (232.5 g/day) came from Table 11-12 of EPA's 2011 Exposure Factors Handbook adjusted to liters per day based on the density of homogenized milk at 20°C (1.029 kg/L). Milk concentration came from Clark *et al.* (2011).

Clark *et al.,* (2011) noted that for the low molecular weight phthalates (like DMP), biomarker studies provide a better estimate of intake than do intake studies. Several different biomarker studies specific to data collected in the United States are summarized. They provide estimated geometric mean intakes ranging from 0.021 to 0.034 µg/kg-day, based on a study from the CDC (2005), using data from the NHANES database (2001-2002). These biomarker studies provide additional evidence that general population exposure to DMP is extremely low (*i.e.*, negligible) relative to the RfD of 10,000 µg/kg-day. Other intake-based exposure estimates for the U.S. summarized in Clark *et al.,* (2011) range from 0.05 to 1.6 µg/kg-day as median values, which further demonstrate that exposure is negligible compared to the 10,000 µg/kg-day RfD. Based on the available information, it seems that the exposure to dimethyl phthalate for the general population is very low.

Selenium

Background

Selenium (CASRN 7782-49-2) is classified as a naturally occurring, solid metalloid substance within the earth's crust, rocks, and soil (IPCS, 1987). Distribution of selenium varies regionally and it is found more commonly at higher concentrations in drier regions of the western and mid-western United States (ATSDR, 2003). In the environment, pure elemental selenium is rare, while selenium compounds incorporating substances such as oxygen and sulfides predominate. According to the ATSDR (2003), selenium is produced commercially, primarily as a byproduct of copper refining.

Selenium is also found in a wide range of consumer products such as plastics, paints, dietary supplements and anti-dandruff shampoos and is important to a wide variety of industries including electronic, pharmaceutical, and agricultural sectors (Barceloux, 1999).

Selenium is an essential micronutrient supporting human life and primary exposure occurs orally through food-based consumption followed by water intake and air exposure (Barceloux, 1999). Environmental processes such as weathering and erosion play a role in the distribution of selenium in the environment. These processes lead to the dispersion of airborne particulate matter/ aerosols and deposition of selenium into waterways which has the capacity to promote subsequent vegetative uptake and/or bioaccumulation in aquatic species. Sodium selenate is the most water soluble selenium species (ATSDR, 2003). Anthropogenic release triggered by activities such as the burning of coal discharges selenium compounds to the atmosphere. According to the OEHHA (2010), selenium has the capacity to exist in three distinct states within the atmosphere: the vapor phase, as a gas, or as a component of precipitation. The mobility and ultimate fate and transport of selenium and selenium compounds within soils is reliant on soil acidity and oxygen interactions (ATSDR, 2003). Dose and responses to selenium exposures are also influenced by factors such as profession/occupational setting, dietary consumption patterns, and place of residence.

Exposure Source Determinations

Manufacturing and release

Release of selenium to the environment is generated through anthropogenic and natural sources. Many sectors utilize selenium and/or selenium-based compounds as a component of their manufacturing processes including applications such as manufacturing of ceramics, steel, vulcanization of rubber, and the production of pigments (Barceloux, 1999). According to the USEPA's Chemical Data Access Tool (CDAT) 4 producers in the United States have a national production volume of selenium ranging from 500,000 to 1,000,000 lbs selenium/year and each have past production volumes of over 100,000 lbs selenium/year (USEPA, 2013F).

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[17] of selenium in 2011 accounted for

[17] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[18] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

309,679.87 pounds with the majority of release/disposal occurring through RCRA Subtitle C landfills, point source air emissions, and fugitive air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[18] in 2011 accounted for 82,647.44 pounds of selenium with the majority of disposal/release occurring through "other landfills" and "other land disposal" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for selenium in 2011 was 392,327.31 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 232,595.80 pounds of selenium with the majority of disposal/release occurring through RCRA Subtitle C landfills and point source air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 49,984.96 pounds selenium with the majority of disposal/release occurring through "other land disposal" and solidification/stabilization (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for selenium in 2012 was 282,580.76 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

Selenium concentrations in treated/municipal drinking water tend to be very low. The U.S. EPA has established a Maximum Contaminant Level (MCL) for selenium in drinking water of 0.05 mg/L (US EPA, 2012B). According to the ATSDR (2003) in 99.5% of drinking water sources tested, selenium levels were less than 10 µg/L. According to the United States Environmental Protection Agency, selenium concentrations in trace amounts ranging from non-detect to 0.01 mg/L are routinely found in drinking water (USEPA, N.D.). For the purposes of RSC calculation a value of 0.01 mg/L of selenium in treated drinking water was used. A standard drinking water intake of 2.0 L/day and a standard body weight of 70 kg were also utilized in this calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of selenium received through ingestion of treated drinking water was 2.86 $x10^{-4}$ mg/kg-day.

Groundwater

In select cases, groundwater wells in seleniferous areas of the United States seem to possess higher levels of selenium. Seleniferous soils and areas that are susceptible to selenium contamination in water bodies due to mobilization from soils are concentrated in the Western United States. Underlying geology that influences the composition of parent materials generated from bed rock and evaporative indexes influence susceptibility to selenium contamination (USGS, 1997). The Eastern United States have evaporative indexes of less than 2.0 making selenium contamination through this pathway negligible (USGS, 1997). However, in combination with their underlying geology, the Western United States have evaporative indexes greater than 2.5, thus putting states

such as Texas, North Dakota, Oklahoma, Kansas, South Dakota, New Mexico, Colorado, Wyoming, Montana, Utah, California, and Arizona at much higher risk of selenium contamination in water bodies generated from soil mobilization (USGS, 1997). Agricultural drainage has been shown to increase selenium levels in groundwater in low lying areas (Su *et al.,* 2007). Moreover, processes involved in natural gas extraction have been shown to increase selenium levels in private wells in the north Texas area (Fontenot *et al.,* 2013). Thus, geochemical processes and anthropogenic activities possess the potential to influence and increase selenium concentrations in drinking water above trace amounts that are not expected to generate adverse effects coinciding with exposure, especially when pumped from well-based systems.

Air

Multiple sources provided a range of recordings of atmospheric selenium concentrations. According to the ATSDR (2003) exposure to ambient air through the inhalation pathway is minimal due to the fact that ambient air concentrations are generally less than 10 ng/m^3. As documented by the World Health Organization (2011), Zoller and Reamer (1976) conducted a study which found that urban air concentrations of selenium ranged from 0.1 to 10 ng/m^3. Dose received through the inhalation exposure route seems to be dependent upon location with respect to proximity to industrial sites such as copper smelters and regions of the world. According to U.S. EPA's 2005 National Air Toxics Assessment data, the total ambient selenium concentration for the state of Florida was 9.69 x 10^{-5}µg/ m^3 (USEPA, 2005A). In Birmingham, Alabama from 2005 to 2006, a large-scale air toxics study was conducted for chemicals of concern. For each of the four study sites which were noted for their industrial proximity or proximity to high traffic areas, selenium did not exceed the chronic non-cancer hazard threshold (Jefferson County Health Department, 2009). However, studies in overseas countries such as China and Turkey have shown selenium concentrations in ambient air far exceeding concentrations measured in the United States (ATSDR, 2003; OEHHA, 2010). The majority of selenium found in ambient air is removed by wet and dry deposition (ATSDR, 2003). For the purposes of RSC calculation, a value of 10 ng/m^3 was utilized due to the conservativeness of this estimate. A standard inhalation rate of 16 m^3/day and a standard body weight of 70 kg were also utilized in this calculation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of selenium received through inhalation was 2.29 x10^{-6} mg/kg-day.

Oceanic/ marine levels

Selenium concentrations in sea water range from 0.052-0.50 µg/L (USEPA, 2013B) with an average of 9.0 x 10^{-5}mg/L (0.09 µg selenium/L) (ATSDR, 2003). Higher concentrations are suspected to occur in marine biota due to the accumulative nature of selenium. According to the United States Environmental Protection Agency (N.D.), samples of marine fish meal have been documented to contain selenium concentrations of approximately 2 ppm.

Soil

Adsorption and retention of selenium in soils is dependent on pH, redox conditions within soils and composition of the soil (McLean and Bledsoe, 1992). Selenium becomes more mobile as soil alkalinity increases which positively influences the risk of human exposure (Breckenridge and

Crockett, 1995). According to Su *et al.* (2007), the majority of soils in the United States contain a selenium concentration ranging from 0.1-2.0 mg/kg; however, certain soils generated from Upper Cretaceous marine sedimentary rocks (shale) show regionally elevated selenium concentrations in about 80,000 km^2 of land in the 17 western states of the United States. Additionally, by-products and waste discharges from uranium mills, surface coal mining, and waste rock from phosphate mining have been found to increase soil selenium and subsequently groundwater selenium concentrations (Su *et al.*, 2007). According to the ATSDR (2003), a study of over 400 Florida-based surface soil samples revealed selenium concentrations ranged from 0.01–4.62 µg/g and possessed an arithmetic mean selenium concentration of 0.25 µg/g. For the purposes of RSC calculation, the Florida-specific arithmetic mean selenium concentration of 0.25 µg/g was utilized. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized in this calculation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of selenium received through soil ingestion was 1.79 $x10^{-4}$ mg/kg-day.

Diet (other than fresh or estuarine fish)

Dietary consumption of selenium through food sources is considered to be the primary route of exposure with estimated daily intake ranging from 0.071 to 0.152 milligrams (USEPA, 2013G). Many studies have attempted to quantify the selenium content of individual food types. Selenium content is dependent on the type of foodstuff and the place of production of that food source. Selenium is present in many different types of foodstuffs with the highest concentrations in foods with higher protein levels (Finley, 2006). The World Health Organization (2011) suggests the most important dietary sources of selenium are meats and seafood (0.3-0.5 mg/kg) and cereals (0.1-10 mg/kg). The recommended daily allowance for selenium is 55 µg/day for adult males and females (Finley, 2006), 60 or 70 µg/day for pregnant/ lactating women respectively, 15 µg/day for young infants, and 30 µg/day for children between the ages of 4 and 8 years old (WHO, 2011). According to the ATSDR (2003) the Tolerable Upper Intake Level (UL) is 0.4 mg/day for adult-based selenium consumption. According to Bialostosky, *et al.* (2002), NHANES III dietary intake data spanning the years from 1988 to 1994 revealed that the mean selenium intake for the total population sampled was 114 µg/day. The U.S. EPA's Integrated Risk Information System (IRIS) reported the oral reference dose (RfD) for selenium as 0.005 mg/kg-day with a NOAEL of 0.015 mg/kg-day and LOAEL of 0.023 mg/kg-day (USEPA, 2013C). For the purposes of RSC calculation, a value of 114 µg/day was utilized to represent dietary dose due to the conservativeness of the estimate. A standard body weight of 70 kg a day was also utilized in this calculation (USEPA, 1997). The resultant estimated average daily dose of selenium received through dietary intake was 1.63 $x10^{-3}$ mg/kg-day.

Exposures for potentially highly exposed individuals

A number of factors make certain individuals more sensitive to selenium exposure and/or susceptible to receiving higher levels of exposure to selenium than the general public. Individuals living in close proximity to hazardous waste sites or in the western United States which more commonly possess seleniferous soils have the potential to receive higher selenium exposures. Individuals in certain occupations such as coal mining possess the potential to be exposed to greater selenium levels. Diets consisting primarily of locally grown or self-caught foodstuffs in

areas of high selenium concentrations have the potential to receive higher exposure. Children, which have a recommended daily allowance of 30 µg/day, possess a lower threshold for selenium exposure and may be more sensitive to selenium doses that distinguish between deficiency and toxicity.

Ambient Exposure Sources

Aquatic biota have the potential to bioaccumulate selenium within their own tissues and biomagnify selenium concentrations through hierarchical trophic chains (ATSDR, 2003). According to Presser (2010), selenium toxicity arises when dissolved Se is transformed to organic Se after uptake by bacteria, algae, fungi, and plants and then passed through food webs. Selenium levels in the majority of United States surface water bodies are relatively low. As documented by the ATSDR (2003), Lakin and Davidson 1967 conducted a study of selenium concentrations in major watersheds of the United States and detected selenium in only 2 of 535 samples (<0.5%) at a concentration greater than the lowest detection limit of 0.010 mg/L. However, geochemical processes involving the interaction between seleniferous rocks such as shale and ambient waters and agricultural and industrial discharges have the potential to greatly increase selenium concentrations, which adversely affect wildlife populations as seen at Kesterson national wildlife refuge (ATSDR, 2003).

RSC calculation

The estimated doses received through daily exposure to selenium were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 1** below.

Table 1. . Estimated average daily selenium exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg-day)**
Inhalation of Air	2.28571×10^{-6}
Soil ingestion	1.78571×10^{-4}
Treated drinking water ingestion	2.85714×10^{-4}
Diet	1.62857×10^{-3}
Estimated total daily dose	$\mathbf{2.09514 \times 10^{-3}}$

The reference dose for selenium is 0.005 mg/kg-day (USEPA, 2013C). The estimated total non-ambient exposure of 2.095×10^{-3} mg/kg-day represents 41.9% of the RfD. The remaining 58.1% is available for allocation to surface water exposures through routes such as estuarine fish consumption. Thus, a chemical specific RSC of 0.58 is suggested to be protective of human health.

Ethylbenzene

Background

Ethylbenzene is an aromatic hydrocarbon naturally present in crude petroleum. It is also a combustion byproduct of biomass. It is widely distributed in the environment because of human activities such as the use of fuels and solvents (which account for the bulk of emissions) and through chemical manufacturing and production activities. It is primarily used for the production of styrene, which is the monomeric unit for polystyrene materials. Ethylbenzene is also used as a solvent and in the manufacture of several organic compounds other than styrene; however, these uses are very minor in comparison to the amounts used for styrene production. Consumer products containing ethylbenzene include gasoline, paints, inks, pesticides, carpet glues, varnishes, paints, tobacco products, and other automotive products. The production volume of ethylbenzene is typically among the highest of all chemicals manufactured in the United States. In 2005, nearly 12 billion pounds of ethylbenzene were produced domestically, with historical levels ranging anywhere from approximately 7 to 13 billion pounds annually (ATSDR, 2010). Routine human activities, such as driving automobiles, boats, or aircraft, and using gasoline-powered tools and equipment as well as paints, varnishes, and solvents release ethylbenzene to the environment.

Environmental and background levels of ethylbenzene are generally small and therefore, have minimal impact on public health. Trace levels of ethylbenzene are found in internal combustion engine exhaust, food, soil, water, and tobacco smoke, but usually at levels well below those that have been shown to exhibit toxic effects in laboratory animals or human exposure studies (ATSDR, 2010). Ethylbenzene is not considered highly persistent in the environment. It partitions primarily to air and removal via photochemically generated hydroxyl radicals is an important degradation mechanism. The half-life for this reaction in the atmosphere is approximately 1–2 days. Biodegradation under aerobic conditions and indirect photolysis are important degradation mechanisms for ethylbenzene in soil and water. Based on a vapor pressure of 9.53 mm Hg and Henry's law constant of 7.9×10^{-3} atm-m^3/mol, volatilization from water and soil surfaces is expected to be an important environmental fate process for ethylbenzene. If released to soil, ethylbenzene is expected to possess moderate mobility based on a soil adsorption coefficient (Koc) value of 240.

Ethylbenzene tends to partition to the atmosphere when it is released to the environment, due to the compound's volatile nature; therefore, exposure to this chemical is most likely to occur through inhalation. However, it is also present in trace amounts in some water supplies and food items. Thus, ingestion also may be an important exposure pathway in some cases. The general population is primarily exposed to ethylbenzene from the inhalation of ambient air. This is due to the direct release of ethylbenzene into the air by the burning of fossil fuels or industrial processes, and partitioning into the air from other media (*e.g.*, soil, surface water). This partitioning of ethylbenzene into the air or water would play a role in exposure to populations living near hazardous waste sites. In addition to inhalation exposure, ingestion of ethylbenzene may also occur because trace amounts have been found in water supplies and various food items.

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[19] of ethylbenzene in 2011 accounted for 3,511,425.97 pounds with the majority of release/disposal occurring through point source air emissions, fugitive air emissions, and underground injection to Class I wells (TRI2011, 2013A). Total reported off-site disposal or other releases[20] in 2011 accounted for 202,381.35 pounds of ethylbenzene with the majority of disposal/release occurring through "other off-site management" and waste brokers (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for ethylbenzene in 2011 was 3,713,807.31 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 3,431,928.38 pounds of ethylbenzene with the majority of disposal/release occurring through point source air emissions, fugitive air emissions, and underground injection to Class I wells (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 263,944.28 pounds of ethylbenzene with the majority of disposal/release occurring through "other off-site management" and RCRA Subtitle C Landfills (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for ethylbenzene in 2012 was 3,695,872.66 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

Concentrations of ethylbenzene are not frequently detected in treated drinking water supplies. Ethylbenzene is regulated as a VOC in drinking water and all non-purchased community water systems (CWSs) and non-transient non-community water systems (NTNCWSs) are required to sample for VOCs (USEPA, 2009C). In the *Contaminant Occurrence Support Document for Category 2 Contaminants for the Second Six- Year Review of National Primary Drinking Water Regulations,* the

[19] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[20] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

United States Environmental Protection Agency analyzed the reported VOC data from 49,969 public water systems (PWSs) during the period from 1998 to 2005 (USEPA, 2009C). For drinking water originating from ground water sources, a median concentration of 0.9 μg/L and a 90th percentile concentration of 4.4 μg/L were detected (USEPA, 2009C). For drinking water originating from surface water sources, a median concentration of 0.9 μg/L and a 90th percentile concentration of 6 μg/L were detected (USEPA, 2009C). According to the ATSDR (2010), ethylbenzene concentrations of 1.6, 1.8, and 2.3 µg/L were previously detected at drinking water treatment plants in New Orleans, Louisiana. The IPCS (1996) reported a study conducted by Otson *et al.* (1982) which found that ethylbenzene concentrations ranging from less than 1 to 10 µg/L were previously detected in Canadian potable drinking water. The IPCS (1996) also reported a study conducted by Coleman *et al.* (1984) which investigated ethylbenzene concentrations in drinking water from Cincinnati, Ohio and detected a level of 0.036 µg/L. The United States Environmental Protection Agency has established a maximum contaminant level (MCL) of 0.7 mg/L for ethylbenzene (USEPA, 2012A). For the purposes of RSC calculation, an ethylbenzene concentration of 0.7 mg/L was utilized due to the fact that this concentration represents the most conservative estimate of exposure. A standard drinking water intake rate of 2.0 L/day and a standard body weight of 70 kg were also utilized (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of ethylbenzene received through treated drinking water intake was 0.02 mg/kg-day.

Air

The Toxic Release Inventory (TRI) provided an estimated release of 4,586,441 pounds (~2,081 metric tons) of ethylbenzene to the atmosphere from 1,485 domestic manufacturing and processing facilities in 2006 (TRI2006, 2008). These air releases accounted for about 82% of the estimated total environmental releases from facilities required to report to the TRI (TRI2006, 2008). The total atmospheric release from reported Florida facilities during 2006 was 104,231 pounds or 99.7% of ethylbenzene releases in Florida. The TRI data should be used with caution since only certain types of facilities are required to report.

Ethylbenzene evaporates at room temperature and can be detected in ambient air by smell when concentrations reach 2 ppm (ATSDR, 2010). Ambient air levels of volatile organic compounds, including ethylbenzene, were monitored as a part of a multi-media study known as the Lower Rio Grande Valley Environmental Scoping Study. Monitoring was performed at a "central" site and at a "border" site in the Brownsville, Texas, airshed in the spring and summer of 1993. The median ambient concentration of ethylbenzene at the central site was 0.80 µg/m^3 (n=22; range=0.20–1.7 µg/m^3) in the spring and 0.4 µg/m^3 (n=14; range=0.2–1.0 µg/m^3) in the summer. These concentrations are either lower or comparable to those found in previous EPA and other monitoring investigations (Ellenson *et al.*, 1997). The median indoor concentration of ethylbenzene for nine Rio Grande Valley residences measured in the spring was 1.00 µg/m^3 compared to a median outdoor concentration of 0.70 µg/m^3; in the summer, the median indoor concentration of ethylbenzene for five residences was 1.40 µg/m^3 compared to a median outdoor concentration of 0.35 µg/m^3 (Ellenson *et al.*, 1997). The mean indoor concentration of ethylbenzene at the homes of 46 high school students residing in New York City was 3.57 µg/m^3 in the winter months as

compared to a mean indoor concentration of 1.99 µg/m^3 during the summer months (Kinney *et al.* 2002). The corresponding mean outdoor levels of ethylbenzene were 1.27 and 1.88 µg/m^3 in the winter and summer months, respectively. Kim *et al.* (2001), conducted an investigation of VOC concentrations in urban domestic and public microenvironments in Birmingham, United Kingdom. Through the use of adsorbent tubing fitted to a personal pump operated at a flow rate of ca. 40 mL/min concentrations of 15 VOCs, including ethylbenzene, were monitored in homes, offices, laboratories, cinemas, department stores, perfume shops, libraries, pubs, restaurants, train stations, coach stations, trafficked roadside locations, automobiles, buses, and trains. **Table 1** below provides the mean concentrations (µg/m^3) of ethylbenzene in each of the previously mentioned microenvironments.

Table 1. Mean Concentrations of Ethylbenze from the Kim *et al*. (2001) VOC Microenvironment Study.

Type of Microenvironment	Number of Samples Collected	Mean Concentration of Ethylbenzene (µg/m^3)
Homes	64	2.3
Offices	12	2.4
Laboratories	8	0.7
Cinemas	6	5.9
Department stores	8	3.4
Perfume shops	3	2.4
Libraries	6	3.5
Pubs	6	7.3
Restaurants	6	6.2
Train stations	12	7.4
Coach stations	12	3.8
Trafficked roadside locations	12	12.4
Automobiles	35	51.9
Buses	18	8.0
Trains	18	5.6

Emissions and modeled ethylbenzene concentrations were queried from the USEPA National-Scale Air Toxics Assessment http://www.epa.gov/ttn/atw/natamain/index.html (NATA; USEPA, 2013D). NATA is EPA's ongoing comprehensive evaluation of air toxics in the United States. The USEPA developed NATA as a state-of-the-science screening tool for state/local/tribal agencies to prioritize pollutants, emission sources, and locations of interest for further study in order to gain a better understanding of risks. NATA assessments do not incorporate refined information about emission sources, but rather, use general information about sources to develop estimates of risks which are more likely to overestimate impacts than underestimate them. The resulting risk estimates are purposefully more likely to be overestimates of health impacts than underestimates, and thus they are health protective.

FDEP downloaded the most recent NATA results (USEPA, 2005A). Data for all Florida counties were queried from the database http://www.epa.gov/ttn/atw/nata2005/tables.html. The estimated total statewide atmospheric ethylbenzene concentration was 0.281 μg/m^3 from point and non-point sources. Individual county concentrations ranged from 0.0086 μg/m^3 in Lafayette County to 0.461 μg/m^3 in Miami-Dade. The median atmospheric concentration across all counties was 0.088 μg/m^3. The ATSDR (2010) reports that median ethylbenzene concentrations in air in city and suburban locations is 0.62 ppb, 0.01 ppb in rural locations, and 1 ppb for indoor air. To convert these concentrations into a usable format for RSC calculation, the following equation was utilized and then subsequently converted into mg/m^3:

$$\text{Concentration in (ppb)} = \frac{24.45 \text{ x concentration } (\mu g/m^3)}{\text{molecular weight}}$$

*Equation utilized originates from *Understanding units of Measure* (October 2008) which was developed by Terrie K. Boguski, P.E., Assistant Technical Director of the Center for Hazardous Substance Research (CHSR) at Kansas State University.

The molecular weight of ethylbenzene utilized was 106.17 (ATSDR, 2010). Thus, the city/suburban concentration was subsequently calculated to be 2.69 x 10^{-3} mg/m^3, the rural concentration was subsequently calculated to be 4.3 x 10^{-5} mg/m^3, and the indoor air concentration was subsequently calculated to be 4.34 x 10^{-3} mg/m^3. For the purpose of RSC calculation, the median concentration of 2.69 x 10^{-3} mg/m^3 was utilized to represent outdoor air exposure and the concentration of 4.34 x 10^{-3} mg/m^3 was utilized to calculate indoor air exposure to ethylbenzene. In addition, an outdoor inhalation rate of 3.122 m^3/day, an indoor inhalation rate of 12.878 m^3/day and a standard body weight of 70kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of ethylbenzene received through outdoor inhalation was 1.20 x10^{-4} mg/kg-day and the resultant estimated average daily dose of ethylbenzene received through inhalation of indoor air was 7.98 x 10^{-4} mg/kg-day.

Soil

Ethylbenzene is predicted to have moderate mobility in soils. Soils with greater organic matter content are estimated to slow the movement of ethylbenzene through this medium by a minimal amount. When ethylbenzene is introduced to soils that possess a lower organic matter content, ethylbenzene possesses a greater capacity to leach into groundwaters (ATSDR, 2010). Information and data concerning typical concentrations of ethylbenzene detected in soils are scarce. According to the ATSDR's 2011 *ToxGuide for ethylbenzene*, this chemical is rarely detected in soil (ATSDR, 2011). Soukup *et al*. (2007) analyzed ethylbenzene concentrations in contaminated soil samples obtained from the site of a former crude oil and natural gas production facility near Los Angeles, California. Concentrations ranged from the limit of detection (0.005 mg/kg) to 160 mg/kg. For the purposes of RSC calculation, the range of reported soil concentrations from the California study was used. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized in this calculation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose range of ethylbenzene received through soil ingestion was 3.57 x10^{-9} to 1.14 x10^{-4} mg/kg-

day. The upper end of this range represents an extremely unlikely exposure rate for the vast majority of the general population given that it represents a level from a contaminated site and the opinion of the ATSDR that ethylbenzene is at detectable levels in soil. Therefore, the lower estimation, based on the detection limit, was used for RSC computation purposes.

Groundwater

Common sources of ethylbenzene-based groundwater contamination are industrial discharge, fuel leakages, and improper waste disposal. According to the IPCS (1996), concentrations of ethylbenzene in uncontaminated groundwaters are typically less than 0.1 µg/L. Through a collaborative partnership between the USGS and the United States Environmental Protection Agency, national water quality assessment (NWQA) data from the years ranging from 1992-2001 were analyzed for their ethylbenzene content. For ground waters a total of 4,653 samples were taken from 4,153 sites of which 2.3% of samples detected ethylbenzene (USEPA, 2009C). A median ethylbenzene concentration of 0.01 µg/L and a 99th percentile ethylbenzene concentration of 270 µg/L were produced from the groundwater samples under analysis (USEPA, 2009C).

Oceanic/marine levels

As reported by the ATSDR (2010), Gschwend *et al.* (1982) reported a Massachusetts-based average ethylbenzene seawater concentration range of 0.0018–0.022 µg/L (ppb) and Sauer *et al.* (1978) reported an ethylbenzene concentration range of 0.0004–0.0045 µg/L (ppb) detected in the Gulf of Mexico.

Diet (other than fresh or estuarine fish)

Residual concentrations of ethylbenzene are detected in a wide variety of food types. The United States Food and Drug Administration conducted an analysis of pesticide residuals in specific food types through their Total Diet Study program. The information summarized in this analysis pertains to Total Diet Study market baskets 1991-3 through 2003-4 collected between September 1991 and October 2003 (USFDA, 2006). FDEP analyzed each specific food type for reported ethylbenzene concentrations. Each food type was then separated into a distinct category: fruits, vegetables, meats, dairy, grain, fish (non-estuarine), and fats. Foods not included from the analysis were considered to be composite foods (e.g., "taco/tostada with beef and cheese from Mexican carry out"; "quarter pound cheeseburger on bun, fast food"; and "cheese and pepperoni pizza regular crust from pizza carry out") covered by each previously delineated category. Ethylbenzene concentrations for each food category were then averaged and standard intake rates (USEPA, 2011A) were then utilized to calculate doses from exposure to each food group. **Table 2** provides the results of these calculations.

Table 2. Estimated exposure to ethylbenzene through food-based dietary intake.

Food Category	Average Concentration (ppm)	Intake Rate (g/kg-day)	Dose received through Exposure (mg/kg-day)
Fruits	0.000768	1.6	1.23×10^{-6}
Vegetables	0.00141	2.9	1.01×10^{-5}
Meats	0.001424167	2.0	2.85×10^{-6}
Dairy	0.0008425	6.6	5.56×10^{-6}
Fish (non-estuarine)	0.00159	0.22	3.50×10^{-7}
Grains	0.002365	2.6	6.15×10^{-6}
Fats	0.00416	1.2	4.99×10^{-6}

*As per the United States Environmental Protection Agency's 2011 Exposure Factors Handbook (Chapter 14 Total Food Intake) beverages, sugar, candy, and sweets, and nuts (and nut products) were not included because they could not be categorized into the major food groups.

According to the ATSDR (2010), trace concentrations of ethylbenzene have been reported in split peas (0.013 mg/kg [ppm]), lentils (0.005 mg/kg [ppm]), and beans (mean concentration 0.005 mg/kg [ppm]; maximum concentration 0.011 mg/kg [ppm]). These concentrations were factored into the exposure calculation associated with vegetable intake. Ethylbenzene also has the capacity to migrate from polymer-based packaging material containing foodstuffs, subsequently contaminating those foods. The rate of migration of ethylbenzene from food packaging material, predominantly polystyrene depends on the fat content of the food type enclosed in the packaging (Tang *et al.*, 2000). Based upon a literature analysis, Tang *et al.* (2000) estimated the average daily intake of ethylbenzene through diet ranges from 0.01 to 0.03 µg/kg body weight for adults. When converted to µg/kg-day the FDEP estimated dietary exposure using the USFDA Total Diet Study data, the total estimated dietary intake generated is 0.03123 µg/kg-day which lies at the upper end of the range proposed by Tang *et al.* (2000) and is thus considered to be a conservative estimate of dietary exposure.

<u>Exposures for potentially highly exposed populations</u>

Individuals who smoke tobacco-based products could be at a potentially higher risk of ethylbenzene exposure. In addition individuals living in close proximity to high traffic areas, gas stations, petroleum or chemical refineries, or have wells down gradient of leaking gasoline storage tanks could be at a potentially higher risk of ethylbenzene exposure than the general population (ATSDR, 2010).

Ambient Exposure Sources

According to the ATSDR (2010), the United States Environmental Protection Agency has set a recommendation that if you eat fish and drink water from a body of water, the water should contain no more than 0.53 ppm ethylbenzene. The United States Environmental protection Agency conducted a concurrent analysis of NAWQA data from the years 1992-2001, for detections of ethylbenzene in ambient surface waters. For ambient surface waters a total of 1,402 samples were taken from 182 sites of which 17.3% of samples detected ethylbenzene representing 31.3% of the

sites under analysis (USEPA, 2009C). A median ethylbenzene concentration of 0.0132 µg/L and a 99th percentile ethylbenzene concentration of 1.9 µg/L were produced from the ambient surface water samples under analysis (USEPA, 2009C). Based upon an analysis of STORET data, Staples *et al.* (1985) reported that out of 1,101 ambient surface water samples a median concentration of less than 5.0 µg/L was detected.

RSC Calculation

The estimated doses received through average daily exposure to ethylbenzene were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 3** below.

Table 3: Estimated average daily ethylbenzene exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg-day)**
Indoor air inhalation	7.98×10^{-4}
Outdoor air inhalation	1.20×10^{-4}
Soil ingestion	3.57×10^{-9}
Treated drinking water ingestion	0.02
Diet: Vegetables	1.01×10^{-5}
Diet: Fruit	1.23×10^{-6}
Diet: Meats	2.85×10^{-6}
Diet: Fish (non-estuarine)	3.50×10^{-7}
Diet: Dairy	5.56×10^{-6}
Diet: Grains	6.15×10^{-6}
Diet: Fats	4.99×10^{-6}
Estimated total daily dose	**0.0210**

The oral Reference dose (RfD) for ethylbenzene is 1×10^{-1} mg/kg-day (USEPA, 2013C). The estimated non-ambient exposure of 0.021 mg/kg-day represents 20.95% of the RfD. The remaining 79.05% is available for allocation to surface water exposures through routes such as estuarine fish consumption. Estimates of soil concentrations are scarce. However, the literature suggests that ethylbenezene is rarely at detectable levels in soils. The estimated total non-ambient exposure summarized in **Table 3** included an exposure value from soil based on the detection limit from a study conducted at a contaminated site. Using the maximum soil concentration reported from that same study would have had minimal influence on the calculated RSC; the total non-ambient exposure would have been estimated at 21% rather than 20.95% under the most conservative scenario of soil contamination. There is no basis for believing that the general population is exposed at this extreme level. The potential exposure through soil ingestion is minor or even negligible when compared to other routes. Thus, a chemical-specific RSC of 0.79 is suggested to be

protective of human health and representative of ethylbenzene exposures received through ambient sources.

2,4-Dichlorophenol

Background

2,4-Dichlorophenol (CASRN 120-83-2) is a chemical that possesses two chlorines added to an aromatic phenol and exists as a solid at room temperature. 2,4-dichlorophenol is primarily utilized as an intermediate constituent in the production of 2,4-dichlorophenoxyacetic acid which is used in pesticide applications. 2,4-Dichlorophenol is also utilized as a mothproofing agent, germicide, and antiseptic (WHO,2003A). According to the ATSDR (1999), chlorophenols are produced during the chlorination of organic material present in industrial and municipal waste waters. In addition, chlorination of drinking water at treatment plants can result in detectable levels of chlorophenols if the required precursors are available in the raw water (ATSDR, 1999). Exposure to 2,4-dichlorophenol can occur through ingestion of contaminated water (resulting as a byproduct of drinking water chlorination/treatment processes), consumption of contaminated foods, or inhalation of contaminated air. The primary exposure route for the general public is through ingestion of either contaminated water or foods. Sorption, volatilization, degradation, and leaching are the primary processes governing the fate and transport of chlorophenols (ATSDR, 1999). pH also plays an important role in determining the availability and mobility of chlorophenols in soils and water. 2,4-Dichlorophenol is a lipid-soluble substance that is analyzed through a major National Health and Nutrition Examination Survey (NHANES) biomonitoring initiative conducted by the United States Centers for Disease Control and Prevention. According to the CDC's *Fourth National Report on Human Exposure to Environmental Chemicals* (2013) the creatinine-corrected urinary 2,4-dichlorophenol geometric mean concentration for NHANES survey years 2009-2010 was 0.838 μg/g verifying human exposure.

Exposure Source Determinations

Manufacturing and release

2,4-Dichlorophenol is released to the environment through anthropogenic activities, manufacturing, and production. According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[21] in 2011

[21] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[22] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1

accounted for 15,177.07 pounds of 2,4-dichlorophenol with the majority of disposal/release occurring through underground injection to Class I wells and fugitive air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[22] in 2011 accounted for 4,964 pounds of 2,4-dichlorophenol with the majority of disposal/release occurring through underground injection to Class I wells and disposal to RCRA Subtitle C landfills (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for 2,4-dichlorophenol in 2011 was 20,141.07 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases of 2,4-dichlorophenol in 2012 accounted for 276,677.37 pounds with the majority of release/disposal occurring through underground injection to Class I wells and fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 173 pounds of 2,4-dichlorophenol with the majority of disposal/release occurring through RCRA Subtitle C landfills (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for 2,4-dichlorophenol in 2012 was 276,850.37 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

In 1982, the United States Environmental Protection Agency estimated average daily drinking water exposure to chlorophenols, based on concentrations reported for 2,4-dichlorophenol, to be 0.4 µg/day (USEPA, 1982). According to Exon (1984), the highest level of polychlorinated phenols found in drinking water in the United States was 1.4 µg/L and levels ranged downward to 0.06 µg/L. As reported by the ATSDR (1999), the United States Environmental Protection Agency recommends that drinking water concentrations of 2,4-dichlorophenol should not exceed 0.02 ppm, the level at which this chemical can be tasted. To mitigate chemical-specific taste, the U.S. EPA recommends 2,4-dichlorophenol concentrations should not exceed 0.3 ppb. For the purposes of RSC calculation, a 2,4- dichlorophenol concentration of 0.3 ppb (0.3 µg/L) was used to calculate dose received through drinking water due to the fact that it represents the most conservative recommended estimate. A standard drinking water intake rate of 2.0 L/day and a standard body weight of 70 kg were also utilized (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of 2,4-dichlorophenol received through drinking water was 8.57×10^{-6} mg/kg-day.

Groundwater

2,4-dichlorophenol may enter groundwater sources through leaching from landfills, industrial/hazardous waste sites, or through improper disposal. According to the ATSDR (1999),

through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

chlorophenol groundwater contamination will occur if sufficient quantities of the chemical are present to exceed the sorption capacity of the vadose zone saturated soils. Groundwater concentrations of 2,4-dichlorophenol tend to be greater when in close proximity to hazardous waste sites. For example, Forst *et al*. (1993) reported an average 2,4-dichlorophenol concentration of 248 µg/L found in leachate samples from a hazardous waste landfill. However, Beltis *et al*. (1982) reported that samples collected on September 9th, 1980 from an uncontaminated well bordering a US Army installation site in Bristol, RI revealed that the average concentration of 2,4-dichlorophenol was 26 µg/L.

Air

Information and data concerning 2,4-dichlorophenol concentrations in ambient air are scarce. Available literature suggests that 2,4-dichlorophenol exhibits a slow rate of volatilization therefore failing to represent a significant transport/fate process. When detected in ambient air, typical concentrations have been measured in trace amounts. For example, 2,4-dichlorophenol was detected at an average concentration of 1.5 ng/m^3 (0.23 ppt) associated with seven separate rain events that occurred in Portland, Oregon in 1984 (ATSDR, 1999). 2,4-Dichlorophenol has a distinct odor that can be detected in water at a concentration of 0.35 µg/L (ATSDR, 1999). According to the National Air Toxics Information Clearinghouse's (NAITCH) *Report of Federal, State, and Local Air Toxics Activities* (1992), Florida developed and adopted an acceptable annual ambient air 2,4-dichlorophenol concentration of 3.0 µg/m^3. For the purposes of RSC calculation, a 2,4-dichlorophenol concentration of 3.0 µg/m^3 was used to estimate dose received through inhalation due to the fact that this value represents the most conservative estimate. A standard inhalation rate of 16 m^3/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily 2,4-dichlorophenol dose received through inhalation was 6.86 x10^{-4} mg/kg-day.

Soil

It is predicted that 2,4-dichlorophenol occurs in soils as a breakdown product originating from the pesticide-based application of 2,4-dichlorophenoxyacetic acid. Biodegradation of 2,4-dichlorophenol by soil microbes is also expected to occur under aerobic conditions. Photodegradation is also an important degradation pathway influencing the fate of 2,4-dichlorophenol in soils. Data and information concerning average concentrations of 2,4-dichlorophenol in typical soils are scarce. Many of the soil concentrations that could be located were associated with sawmills as an artifact of treatment and processing. For example, according to Kitunen and Salkinoja-Salonen (1990) a 2,4-dichlorophenol concentration of 1200 µg/kg dry soil was detected at an abandoned Finnish sawmill. In addition, Valo *et al*. (1984) reported that 2,4-dichlorophenol concentrations ranging from 10 to 2580 µg/kg were detected in two separate Finnish sawmills that utilized chlorophenolic fungicides.

As per Chapter 62-777, FAC, the Florida Department of Environmental Protection has established a residential direct exposure target soil clean-up level of 190 mg/kg for 2,4-dichlorophenol (FDEP, 2005). For the purposes of RSC calculation, a concentration of 190 mg/kg was used under the

assumption that it represents a highly conservative estimate of potential soil contamination levels. This concentration represents a level above which the state would initiate clean-up protocols and is characterized as a high-end exposure estimate instead of a central tendency. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized in this calculation (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of 2,4-dichlorophenol received through soil ingestion was 1.36 x 10^{-4} mg/kg-day.

Oceanic/marine Levels

Information/data concerning oceanic/marine concentrations of 2,4-dichlorophenol could not be located.

Diet (other than fresh or estuarine fish)

Current information/data concerning dietary exposure or distinct concentrations of 2,4-dichlorophenol in different food types could not be located. At high enough concentrations, 2,4-dichlorophenol has the capacity to alter/taint the taste of foods. 2,4-Dichlorophenol is analyzed in the United States Food and Drug Administration's Total Diet Study/Market Basket Program as a chlorophenoxy acid residue. However concentrations of 2,4-dichlorophenol in foods analyzed were not present in either the 1991-2003 or 2004-2005 Total Diet Study analytical results. Residual 2,4-dichlorophenoxyacetic acid concentrations were detected in grain-based products in both the 1991-2003 and 2004-2005 Total Diet Study analytical results. As previously mentioned, 2,4-dichlorophenol can occur as a breakdown product of 2,4-dichlorophenoxyacetic acid. Exon (1984) reported that polychlorinated phenol levels in foods generally range from 0.01 to 0.04 ppm. For the purposes of RSC calculation, the midpoint (0.025 ppm) of the range mentioned above was used to estimate a typical exposure received through dietary consumption. The upper end of the range was considered, but was determined to be unrealistic for the general population based on information in ATSDR (1999), which notes that although food monitoring data are lacking, exposure to 2,4-dichlorophenol through the ingestion of food is expected to be relatively minor. A standard total food intake rate of 29 g/kg-day was also used (USEPA, 2011A). The resultant estimated average daily dose of 2,4-dichlorophenol received through dietary ingestion was 7.25 x 10^{-4} mg/kg-day.

Ambient Exposure Sources

Upon analysis of U.S. EPA STORET data, Staples *et al.* (1985) determined that 2,4-dichlorophenol was positively detected in 0.4% of 876 ambient water sample reporting stations at a median level of less than 10 ppb. Concentrations of 2,4-dichlorophenol have also been detected in storm water run-off ranging from 0.00019 to 0.0032 mg/L (Wilson *et al*. 1992).

Significant bioaccumulation of 2,4-dichlorophenol in fish species is not expected to occur due to rapid metabolism and excretion (ATSDR, 1999). According to the U.S. EPA (1982), maximum exposure through consumption of fish was estimated to be 26 µg/day for 2,4-dichlorophenol.

RSC Calculation

The estimated doses received through daily exposure to 2,4-dichlorophenol were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 1** below.

Table 1: Estimated average daily 2,4-dichlorophenol exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg-day)**
Inhalation of air	6.86×10^{-4}
Soil ingestion	1.36×10^{-4}
Treated drinking water ingestion	8.57×10^{-6}
Diet	7.25×10^{-4}
Estimated total daily dose	1.55×10^{-3}

The reference dose for 2,4-dichlorophenol is 3×10^{-3}mg/kg-day. The estimated exposure is likely to be highly conservative and is greater than estimates provided by the IPCS (1989). The IPCS estimates, for a 70 kg individual, exposure ranged from 3.14×10^{-5} mg/kg-day based on diet and drinking water exposures to 5.71×10^{-5} mg/kg-day assuming indoor rooms were treated with a chlorophenol preservative. The estimated total non-ambient exposure of 1.53×10^{-3} mg/kg-day represents 52% of the RfD. The remaining 48% is available for allocation to surface water exposures through routes such as estuarine fish consumption. Thus, a chemical specific RSC of 0.48 is proposed to be protective of human health and representative of 2,4-dichlorophenol exposures received through ambient sources.

2-Chlorophenol

Background

2-Chlorophenol (CASRN 95-57-8) is a yellow-brown chemical that exists as a liquid at room temperature and possesses a distinct odor. The odor threshold for 2-chlorophenol is 10 µg/L and the taste threshold is 0.1 µg/L (WHO, 2003A). The primary applications of 2-chlorophenol are as a precursor in the production of higher chlorophenols and dyestuffs and as a preserving agent. According to the USEPA (1980B), 2-chlorophenol is slightly soluble at a neutral pH. Microbial degradation is predicted to play a role as a 2-chlorophenol degradation pathway. Due to the fact that 2-chlorophenol is used almost exclusively as an intermediate in the production of other chemicals, there is a greater risk associated with exposure to individuals occupationally involved with 2-chlorophenol than the general public. Exposure to the general population is most likely to occur through the consumption of contaminated foods or contaminated drinking water which contains chlorophenols as a byproduct of disinfection or deodorization.

Exposure Source Determinations

Manufacturing and release

Little information is available concerning the manufacturing and release of 2-chlorophenol. According to the ATSDR (1999) monochlorophenol concentrations ranging from 10-20 µg/L have been released in waste water produced during the manufacture of specialty chemicals. 2-chlorophenol has also been reported but not quantified in municipal landfill leachate and runoff from 1 of 15 cities under analysis by Cole *et al.* (1984).

Non-Ambient Exposure Sources

Treated drinking water

Chlorophenols are present in drinking-water as a result of the chlorination of phenols, as by-products of the reaction of hypochlorite with phenolic acids, as biocides or as degradation products of phenoxy herbicides. According to the ATSDR (1999), the United States Environmental Protection Agency recommends that drinking water concentrations of 2-chlorophenol should not exceed 0.04 parts per million (ppm), the level at which this chemical can be tasted in drinking water. To mitigate chemical-specific taste, the U.S. EPA recommends that 2-chlorophenol concentrations in drinking water should not exceed 0.1 ppb. A study of Canadian potable water treatment facilities conducted in summer revealed a maximum 2-chlorophenol concentration of 65 ng/L (ATSDR, 1999). For the purposes of RSC calculation, a 2-chlorophenol concentration of 0.1 ppb was utilized to estimate exposure through drinking water intake. A standard drinking water intake rate of 2.0 L/day and a standard body weight of 70 kg were also utilized in the calculation (NRC, 1977; USEPA, 1997). The resultant estimated average daily dose of 2-chlorophenol received through drinking water ingestion was 2.86×10^{-6} mg/kg-day.

Air

Typical concentrations of 2-chlorophenol found in ambient air could not be located. The ATSDR (1999) reports of a train derailment and rupture of a train tanker that led to accidental release and subsequent 2-chlorophenol air concentrations ranging from 0.02 to 0.7 mg/m^3. Eighteen days after the spill, air levels were <2 µg/m^3. A conservative estimate of inhalation exposure was calculated using the post spill air level of <2 µg/m^3, daily inhalation rate of 16 m^3/day, and a standard body weight of 70kg (ATSDR, 1999; USEPA, 2011A; USEPA, 1997). The calculated daily exposure was $<4.57 \times 10^{-4}$ mg/kg-day. The representativeness of this value of typical exposures to the general population is unknown. The value is based on information from a single unusual event and actually represents the detection limit rather than a measured concentration. Therefore, this value most likely represents an overestimate of exposure.

Soil

Data and information concerning typical concentrations of 2-chlorophenol found in soils is scarce. Concentrations of 2-chlorophenol ranging from 1.1 to 12,350 µg/kg were detected in soil at 12 different Ville Mercier sites in Quebec, Canada (Valo *et al*., 1984). As per Chapter 62-777, FAC, the Florida Department of Environmental Protection has established a residential direct exposure soil clean-up target level of 130 mg/kg for 2-chlorophenol (FDEP, 2005). For the purposes of RSC calculation, a 2-chlorophenol concentration of 130 mg/kg was utilized under the assumption that it represents a highly conservative estimate of potential soil contamination levels. It represents a level above which the state would initiate clean-up protocols and is characterized as a high end

exposure instead of a central tendency. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of 2-chlorophenol received through soil ingestion was 9.29 x10^{-5} mg/kg-day.

Diet (other than fresh or estuarine fish)

Information and data could not be located concerning 2-chlorophenol concentrations associated with total food intake or concentrations associated with specific food types. However, the literature strongly suggests that monochlorophenols such as 2-chlorophenol do not biomagnify and have short biological half-lives (ATSDR, 1999). Veith *et al.* (1980) reported a half-life of less than one day in bluegill sunfish exposed to 2-chlorophenol. Therefore, dietary exposure from sources other than fresh and estuarine fish for the majority of the general population are expected to be insignificant and were therefore considered negligible for purposes of RSC calculation.

Ambient Exposure Sources

Chlorophenol concentrations in sediments are generally greater than those in the overlying water. Photolysis and microbial degradation of 2-chlorophenol are expected to be significant degradation pathways (ATSDR, 1999). With respect to bioaccumulation potential, a bioconcentration factor was found only for the blue gill and was determined to be 214 with a rapid depuration rate and a half-life of less than one day (USEPA, 1980B). Monochlorophenols at concentrations ranging from 2 to 20 µg/L were found in surface waters in the Netherlands (Piet and Grunt, 1975). According to the USEPA STORET database, of 814 samples, 0.2% tested positive, median concentration of <10 ppb (Staples *et al*., 1985)

RSC Calculation

The estimated doses received through daily exposure to 2-chlorophenol were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 1** below.

Table 1: Estimated average daily 2-chlorophenol exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg-day)**
Inhalation of Air	<4.57 x 10^{-4}
Soil ingestion	9.29 x10^{-5}
Treated drinking water ingestion	2.86 x 10^{-6}
Diet	Negligible
Estimated total daily dose	**<5.53 x 10^{-4}**

The oral Rfd for 2-chlorophenol is 5 x 10^{-3}mg/kg-day (USEPA, 2013C). The estimated exposure from non-surface water sources was calculated to account for less than 11 percent of the 2-chlorophenol reference dose. However, the estimated exposure was calculated based on limited data or surrogate estimates (*i.e*., drinking water); therefore, it only serves as one line of evidence

supporting an RSC. DEP also considered the fact that 2-chlorophenol, like most chlorophenols, exhibits objectionable taste and odor at very low concentrations. The ATSDR (1999) noted that potential exposure, for the general population, to chlorophenols tends to be limited because of the pronounced odor and taste imparted by the presence of these substances. Taste and odor thresholds for 2-Chlorophenol have been noted in the range of 2 to 4 ppb and have been noted to affect the flavor of fish at concentrations of about 2 to 43 times lower than the odor thresholds for these compounds in water. Thus, it is highly unlikely that the general population is exposed to significant levels of the compound. An RSC of 0.8 (EPA ceiling) was selected based on a consideration of both the characteristics of the compound (*i.e.*, objectionable taste and odor) and the estimated low total non-ambient exposure.

2,4-Dimethylphenol

Background

2,4-Dimethylphenol (CASRN 105-67-9) is a naturally occurring substituted phenol derived from the cresol fraction of petroleum or coal tars (USEPA, 1980C). This chemical has a wide variety of applications as a solvent, insecticide, plasticizer, additive in gasoline and lubricants, constituent in pharmaceutical products, and is important to commercial, industrial, and agricultural sectors (US EPA, 1980C). 2,4-Dimethylphenol possesses a distinct odor threshold recognizable in air at a concentration of 0.001 mg/m^3, detectable in air at concentrations ranging from 0.0005 to 0.4 mg/m^3, and detectable in water at concentrations of 0.4 mg/L (Spectrum Laboratories, N.D.) According to the Hazardous Substances Data Bank (HSDB; No. 4253), the general public may be exposed to 2,4-dimethylphenol through inhalation of ambient air influenced by probable sources such as tobacco smoke and automobile exhaust, consumption of foods contaminated with 2,4-dimethylphenol, or through contact with 2,4-dimethylphenol containing products.

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[23] in 2011 accounted for 36,036.62

[23] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[24] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

pounds of 2,4-dimethylphenol with the majority of disposal/release occurring through underground injection to Class I wells and point source air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[24] in 2011 accounted for 516 pounds of 2,4-dimethylphenol with the majority of disposal/release occurring through disposal to RCRA Subtitle C landfills and "other landfills" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for 2,4-dimethylphenol in 2011 was 36,552.62 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases of 2,4-dimethylphenol in 2012 accounted for 48,207.38 pounds with the majority of release/disposal occurring through underground injection to Class I wells and point source air emissions (TRI2013, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 525 pounds of 2,4-dimethylphenol with the majority of disposal/release occurring through RCRA Subtitle C landfills and storage only (TRI2013, 2013B). The total reported on- and off-site disposal or other releases for 2,4-dimethylphenol in 2012 was 48,732.38 pounds (TRI2013, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient sources of exposure

Treated drinking water

Information and/or data concerning 2,4-dimethylphenol concentrations typically detected in treated drinking water could not be located. 2,4-dimethylphenol has been qualitatively identified in drinking water in the United States and detected in 5 finished drinking water samples in the 1970's (HSDB, No.4253).

Groundwater

Groundwater concentrations of 2,4-dimethylphenol are often strongly influenced by industrial discharge and manufacturing byproduct release. Many of the of 2,4-dimethylphenol concentrations reported for groundwater are associated with wood-preserving plants and pine tar manufacturing. For example, Cabot/Koppers an NPL superfund site located in Gainesville, FL, was the site of former wood treating/pine-tar manufacturing and charcoal production facilities and experienced groundwater detection hits for 2,4-dimethylphenol. According to McCreary *et al.* (1983), 10 of 11 wells underlying a former pine-tar manufacturing facility in Gainesville, FL were found to contain 2,4-dimethylphenol ranging in concentration from 1-9400 µg/L (including 2,5-dimethylphenol). Through their analysis of groundwater contamination surrounding United States superfund sites Canter *et al*. (1994) detected a 2,4-dimethylphenol concentration of 110 µg/L in their Biscayne, FL Aquifer study area. By comparison, 2,4-dimethylphenol concentrations are typically lower in areas not in close proximity to these types of sites. For example, Beltis *et al.* (1982) reported detecting a 2,4-dimethylphenol concentration of 26 µg/L from samples collected at an uncontaminated well bordering a US Army installation site in Bristol, RI during September of 1980.

Air

2,4-Dimethylphenol is expected to exist solely in the vapor phase in the ambient atmosphere. Information and/or data concerning 2,4-Dimethylphenol concentrations typically detected in ambient air could not be located.

Soil

Biodegradation by soil microbes and volatilization from most soils are predicted to be important degradation/loss pathways for 2,4-dimethylphenol (HSDB, No. 4252). As per Chapter 62-777, FAC, the Florida Department of Environmental Protection has established a residential direct exposure soil clean-up target level of 1300 mg/L for 2,4-dimethylphenol (FDEP, 2005).

Diet (other than fresh or estuarine fish)

Information and data could not be located concerning 2,4-dimethylphenol concentrations associated with total food intake or concentrations associated with specific food types.

Exposures for potentially highly exposed individuals

Individuals who smoke cigarettes and/or marijuana may be at higher risk of 2,4-dimethylphenol exposure.

Ambient Exposure Sources

Volatilization from surface waters is considered an important loss pathway for 2,4-dimethylphenol based upon its Henry's Law Constant of 1.7 x 10^{-5} atm-cu m/mole (HSDB, No. 4253). A bioconcentration factor of 150 was estimated in the bluegill sunfish which potentially indicates a moderate ability to bioaccumulate in aquatic biota (HSDB, No. 4253). According to Staples *et al.* (1985), upon STORET analysis, 2,4-dimethylphenol was detected in 1% of 804 samples.

RSC Calculation

The oral Rfd for 2,4-dimethylphenol is 2 x10^{-2} mg/kg-day (USEPA, 2013C). An RSC of 0.2 (EPA floor) was used for 2,4-dimethylphenol due to the unavailability of scientific literary-based evidence and data specific to 2,4-dimethylphenol concentrations in environmental media and food stuffs.

2,4-Dinitrophenol

Background

2,4-Dinitrophenol (CASRN 51-28-5) is an anthropogenically-produced organic chemical that possesses a yellowish coloring and exists as a solid at room temperature. 2,4-Dinitrophenol is used primarily in the synthesis of dyes, picric acid, picramic acid, wood preservatives, photographic developers, explosives, and insecticides (ATSDR, 1995C). 2,4-Dinitrophenol was also used as a weight loss drug in the 1930s, but was discontinued in 1938 because of reported adverse effects. 2,4-Dinitrophenol was labeled extremely dangerous and not fit for human consumption by the Federal Food, Drug, and Cosmetics Act of 1938 (Grundlingh and Dargan, 2011). Exposure of the general population to 2,4-dinitrophenol can occur through consumption of contaminated foods or drinking water, inhalation of contaminated air or by contact with contaminated soils.

Exposure Source Determinations

Manufacturing and release

2,4-Dinitrophenol is released to the environment through anthropogenic use, manufacturing and production. According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[25] in 2011 accounted for 14,324 pounds of 2,4-dinitrophenol with the majority of disposal/release occurring through point source air emissions and surface water discharges (TRI2011, 2013A). Total reported off-site disposal or other releases[26] in 2011 accounted for 60 pounds of 2,4-dinitrophenol with the majority of disposal/release occurring through "other land disposal" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for 2,4-dinitrophenol in 2011 was 14,384 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases of 2,4-dinitrophenol in 2012 accounted for 7,658.07 pounds with the majority of release/disposal occurring through point source air emissions and surface water discharge (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 73 pounds of 2,4-dinitrophenol with the majority of disposal/release occurring through "other land disposal" (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for 2,4-dinitrophenol in 2012 was 7,731.07 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Air

Manufacturing and processing, automobile exhaust, the use of 2,4-dinitrophenol-based pesticides, and combustion of hazardous waste containing 2,4-dinitrophenol facilitate the release of this chemical to the atmosphere. In addition, dinitrophenols also form from the atmospheric reactions between benzene and NO_x in ambient air (ATSDR, 1995C). 2,4-Dinitrophenol is expected to exist solely as a vapor in ambient air and is susceptible to photolysis by contact with sunlight (HSDB, No.

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[25] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[25] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

529). Data concerning 2,4-dinitrophenol concentrations in ambient air are scare. 2,4-Dinitrophenol concentrations ranging from 0.1 ng/m^3 to 0.54 ng/m^3 have been reprted in Great Dun Fell, Germany (Luttke and Levsen, 1997). According to the U.S. EPA's 2005 National Air Toxics Assessment data, the total ambient 2,4-dinitrophenol concentration for the state of Florida was 2.00986 x10^{-10} µg/ m^3(USEPA, 2005A). For the purposes of RSC calculation, an ambient air concentration of 2.00986 x10^{-10} µg/ m^3 was utilized because this value represents the most current Florida-based 2,4-dinitrophenol air concentration that could be located. A standard inhalation rate of 16 m^3/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of 2,4-dinitrophenol received through inhalation was 4.59 x10^{-14} mg/kg-day, which is predicted to be a minimal if not negligible exposure to the general population, was subsequently generated.

Treated drinking water

Information/data concerning 2,4-dinitrophenol concentrations typically detected in treated drinking water supplies could not be located.

Groundwater

Industrial discharge and run-off from agricultural applications of 2,4-dinitrophenol based pesticides have the capacity to leach through soils and contaminate groundwaters. According to the ATSDR (1995C), the amount of dinitrophenol leached depends on the dinitrophenol adsorption capability of soils. Adsorption of phenols in soil increases with a decrease in pH and an increase in organic carbon, goethite (one of the most common iron oxides in soil), and clay content. Canter *et al*. (1994) detected 2,4-dinitrophenol in the Biscayne Aquifer at 14 µg/L.

Soil

The fate of 2,4-dinitrophenol in soil is often dependent on the soil characteristics. According to Kaufman (1976), the mobility of dinitrophenols in soils is inversely related to parameters such as acidity, clay, and organic matter content moving slower through soils as these parameters increase. Pakdel *et al.* (1992) detected 2,4-dinitrophenol at a concentration of 11.7 µg/kg in the soil of Ville Mercier, Quebec, Canada. As per Chapter 62-777, FAC, the Florida Department of Environmental Protection established a residential direct exposure soil clean up target level of 110 mg/kg for 2,4-dinitrophenol (FDEP, 2005). For the purposes of RSC calculation, a 2,4-dinitrophenol concentration of 110 mg/kg was utilized under the assumption that it represents a highly conservative estimate of potential soil contamination levels. It represents a level above which the state would initiate clean-up protocols and is characterized as a high end exposure instead of a central tendency. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A, USEPA, 1997). The resultant estimated average daily dose of 2,4-dinitrophenol received through soil ingestion was 7.86 x10^{-5} mg/kg-day.

Diet

Information and data could not be located concerning 2,4-dinitrophenol concentrations associated with total food intake or concentrations associated with specific food types.

Ambient Exposure Sources

According to Callahan *et al.* (1979), significant losses of 2,4-dinitrophenol from surface water are not predicted to occur through volatilization. Instead, biodegradation is predicted to be the most important degradation/loss pathway for 2,4-dinitrophenol in surface waters. Upon analysis of 2,4-dinitrophenol data monitored at U.S. EPA STORET stations, Staples *et al.* (1985) found that 0.4% of the 812 ambient water samples positively detected 2,4-dinotrophenol. The United States Environmental Protection Agency recommends that not more than 70 ppb be present in lakes or streams used for swimming where water may be swallowed (ATSDR ToxFAQs, 1996A). The USEPA also recommends that a dinitrophenol concentration of 0.765 mg/L should not be exceeded in waters where people catch fish to eat, but there is no swimming (ATSDR, 1995C). Bioaccumulation of dinitrophenols in fish is not predicted to occur.

RSC Calculation

The estimated doses received through daily exposure to 2,4-dinitrophenol were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 1** below.

Table 1: Estimated average daily 2,4-dinitrophenol exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg-day)**
Inhalation of Air	4.59×10^{-14}
Soil Ingestion	7.86×10^{-5}
Drinking Water Ingestion	No Information Located
Diet	No Information Located
Estimated total daily dose	**Insufficient Information**

The oral Rfd for 2,4-dinitrophenol is 2×10^{-3}mg/kg-day (USEPA, 2013C). The exposure routes that were able to be quantified represent less than 4% of the 2,4-dinitrophenol reference dose. However, exposure and contamination level data are lacking for both drinking water and dietary exposure routes. Therefore, an RSC of 0.2 (EPA floor) was used for 2,4-dinitrophenol due information adequacy considerations.

2-Methyl-4,6-Dinitrophenol

Background

2-Methyl-4,6-Dinitrophenol (CASRN 534-52-1) also known as 4,6-Dinitro-o-cresol (DNOC) is the most commercially important dinitrocresol isomer. 4,6-dinitro-o-cresol is a non-systemic stomach poison and was formerly utilized as a contact insecticide until 1991 when the United States Environmental Protection Agency canceled its registration as a pesticide agent (ATSDR, 1995B). DNOC is strongly phytotoxic and has been limited to dormant sprays for insecticide-based applications commonly utilized on fruit trees and use as a contact herbicide that was frequently utilized to extricate broad-leaved weeds interspersed in agricultural crops (ATSDR, 1995B).

According to the IPCS (2000), the primary use of DNOC has shifted to the plastics industry as an inhibitor of polymerization in styrene and vinyl aromatic compounds, although still used as a pesticide in a number of other countries. The main source of exposure individuals would have had to 4,6-dinitro-o-cresol was through contact during manufacturing processes and agricultural use such as herbicide application. Volatilization of DNOC is not predicted to be a significant loss pathway for soil or water. According to the ATSDR (1995B), the adsorption of DNOC to soil increases with a decrease in soil pH and an increase in clay and organic carbon contents of soil thus ultimately influencing mobility.

Exposure Source Determinations

Manufacturing and release

According to USEPA Toxic Release Inventory (TRI) data for 2011 and 2012 one cement corporation located in Logansport, Indiana reported their 4,6-Dinitro-O-Cresol waste production (TRI2011, 2013A; TRI2012, 2013B).

Non-ambient Exposure Sources

Environment Canada has completed an assessment of DNOC to assess the potential of this chemical to cause undue risk associated with human exposure to this chemical. This study analyzed estimated exposures to air, drinking water, and soil as quantitative data was not available for DNOC concentrations in food items.

Air

Measured and reported concentrations of DNOC in ambient air are scarce. One of the main routes through which DNOC is released to ambient air is the application of this chemical as a pesticide. DNOC also forms in the atmosphere when 2-methylphenol reacts with NO_x present in ambient air (Leuenberger *et al.,* 1988). To calculate the general population's exposure through inhalation of ambient air, the Environment Canada assessment utilized a concentration of 0.05 $\mu g/m^3$. This concentration originated from a study completed by Leuenberger *et al.* (1988) in Switzerland and was derived through the use of a rainwater to air partition coefficient of 5.6×10^4. According to the National Air Toxics Information Clearinghouse's (NAITCH) *Report of Federal, State, and Local Air Toxics Activities* (1992), Florida developed and adopted an acceptable annual ambient air 4,6-dinitro-o-cresol concentration of 0.48 $\mu g/m^3$ based on a 24 hour averaging time. For the purposes of RSC calculation, an ambient air concentration of 0.48 $\mu g/m^3$ was utilized due to the fact that this value represents the most conservative Florida-based estimate that could be located. A standard inhalation rate of 16 m^3/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DNOC recieved through inhalation was 1.10×10^{-4} mg/kg-day. This estimate is predicted to be highly conservative due to the fact that the USEPA canceled 4,6-dinitro-o-cresol's registration as a pesticide agent approximately 22 years ago.

Treated drinking water

The only information on drinking water levels is a Canadian Report based on a very limited dataset. For drinking water exposure, Environment Canada utilized the detection limit of 0.4 µg/L for DNOC

in 19 samples of tap water from Toronto, Ontario in 2002 (Environment Canada/Health Canada, 2009). Information on drinking water is too limited to confidently estimate an exposure for the general population.

Soil

The primary ways DNOC is introduced to soils is through pesticide-based applications from the agricultural sector, runoff, and manufacturing–based release. DNOC exists primarily in the particle phase within the atmosphere and is potentially susceptible to precipitation-based washout which can also lead to the reintroduction of DNOC to soils. The length of time DNOC is predicted to persist is influenced by underlying soil characteristics and can range from 14 days to greater than l month (ATSDR, 1995B). Environment Canada chose to utilize the method detection limit of 100 ng/g to calculate estimated DNOC exposure through soil ingestion. As per chapter 62-777, FAC the Florida Department of Environmental Protection has established a residential direct exposure soil clean-up target level of 8.4 mg/kg. For the purposes of RSC calculation, the concentration of 8.4 mg/kg was utilized under the assumption that it represents a highly conservative estimate of potential soil contamination levels. This concentration represents a level above which the state would initiate clean-up protocols and is characterized as a high end exposure instead of a central tendency. A standard soil ingestion rate of 50 mg/day and a standard body weight of 70 kg were also utilized (USEPA, 2011A; USEPA, 1997). The resultant estimated average daily dose of DNOC received through soil ingestion was 6.0×10^{-6} mg/kg-day.

Diet (other than fresh or estuarine fish)

Information and data could not be located concerning 4,6-dinitro-o-cresol concentrations associated with total food intake or concentrations associated with specific food types.

Ambient Exposure Sources

Volatilization of DNOC is estimated to be a minimal if not a negligible degradation pathway (ATSDR, 1995B). Various DNOC concentrations detected in surface water bodies were reported with the primary source of contamination noted as influences from run-off through DNOC-based agricultural applications. According to, Klecka *et al.* (2010) summary statistics for the concentrations of pesticides in surface waters from three US systems that border the Great Lakes list 4,6-dinitro-o-cresol as detected in 98% of 165 samples with a 50th percentile concentration of 0.06 µg/L and minimum and maximum concentrations of 0.002 µg/L and 0.190 µg/L, respectively. Hall *et al.* (1987) also reported DNOC concentrations detected in the Potomac River near Quantico, Virginia of less than 10 µg/L. IPCS (2000) reported that DNOC is not expected to bioaccumulate in aquatic organisms due to a rapid degradation time. According to Environment Canada/Health Canada (2009), DNOC readily forms water-soluble sodium, potassium, and ammonium salts and virtually 100% of dissolved DNOC will be in the ionized form at environmentally relevant pHs (pH 6-8).

RSC Calculation

The estimated doses received through daily exposure to 2,4-dinitrophenol were then utilized to estimate the total average daily dose received by the general population. The results are summarized in **Table 1** below.

Table 1. Estimated average daily 2-methyl-4,6-dinitrophenol exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg-day)
Inhalation of Air	1.10×10^{-4}
Soil ingestion	6.0×10^{-6}
Treated Drinking Water ingestion	Limited Information
Diet	No Information Located
Estimated total daily dose	**Insufficient Information**

The reference dose for 2-methyl-4,6-dinitrophenol is 0.00039 mg/kg-day (FDEP, 2013). An RSC of 0.2 (EPA floor) was used for 2-methyl-4,6-dinitrophenol due to the unavailability of scientific literary-based evidence and data specific to 2-methyl-4,6-dinitrophenol concentrations in all environmental media and food stuffs.

Acrolein

Background

Acrolein is a volatile liquid with a burnt, sweet, pungent odor that vaporizes rapidly and easily into the atmosphere, particularly with rising temperatures. It is also a very reactive compound and is highly flammable (IPCS, 1992; ATSDR, 2007). Acrolein is primarily used to make other chemicals, such as acrylic acid and its esters, but may be produced by other sources, including the manufacture of methionine (animal feed supplement), burning of trees and other plants (including tobacco), heating of animal and vegetable fats at high temperatures, and when fossil fuels are burned (IPCS, 1991B; IPCS, 1992; ATSDR, 2007). It is also registered for use as an aquatic biocide in agricultural and industrial water supply systems to control growth of aquatic plants and algae, but only in the western United States (IPCS, 1992; ATSDR, 2007; USEPA, 2008B). When applied to a water body for aquatic plant control, acrolein may persist for as long as six days (ATSDR, 2007).

The primary exposure route for humans is through the air. However, acrolein decomposes into other substances rapidly (within days). Vehicle fuel emissions contain 3 – 10 % of total vehicle exhaust aldehydes. Smoking one cigarette produces between 3 and 228 micrograms of acrolein (IPCS, 1992). Acrolein has not been found in drinking water supplies nor is it common in surface waters (ATSDR, 2007). Acrolein dissolves easily into water, but a significant portion vaporizes to the atmosphere rapidly. Other portions break down in the water column into other substances or bind to solids (ATSDR, 2007). Although the primary exposure pathway is through the air, acrolein levels are very low. However, acrolein levels can be higher in large cities and in environments such as households with people who smoke. In 2007, the ATSDR found that no significant acrolein exposure is expected from ingestion of drinking water or from dermal contact during bathing or showering.

Based on its physical/chemical properties, acrolein is unlikely to partition out of air when released into that medium. Non-pesticidal sources in water, sediment, and soil have not been identified, and acrolein is degraded in these media. Lack of focus on these media is also supported by air monitoring data in Canada and the lack of detectable concentrations of acrolein in water, sediment, and soil. Acrolein does not bioaccumulate in organisms (IPCS, 2002).

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[27] of acrolein in 2011 accounted for 895,283.14 pounds with the majority of release/disposal occurring through underground injection to Class I wells and point source air emissions (TRI2011, 2013A). Total reported off-site disposal or other releases[28] in 2011 accounted for 14 pounds of acrolein with the majority of disposal/release occurring through "other off-site management" and "other landfills" (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for acrolein in 2011 was 895,297.14 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 829,145.79 pounds of acrolein with the majority of disposal/release occurring through underground injection to Class I wells and point source air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for 21.07 pounds of acrolein with the majority of disposal/release occurring through disposal to "other landfills" (TRI2012, 2013B). The total reported on- and off-site disposal or other releases for acrolein in 2012 was 829,166.86 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient exposure sources

Air

[27] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[28] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

Acrolein occurs in the air as a byproduct of volatilization of the liquid, burning of fossil fuels (including vehicle emissions), burning of plant material (e.g., forest fires), cooking fumes, and other sources. The half-life of acrolein in air is estimated to be < 10 hours (Mackay *et al.*, 1995). Other sources (Atkinson, 1985; Grosjean, 1990; USEPA, 2003B; ATSDR, 2007) indicate that the half-life of acrolein in air is estimated to be between 4 – 20 hours.

In the *National Air Quality and Toxics Report, 1998*, the USEPA (2000C) found that concentrations of acrolein in ambient air averaged 0.12 μg/m^3 (rural) and 0.20 μg/m^3 (urban). As reported by the ATSDR (2007), a Canadian study conducted by Environment Canada (2000) estimated that the general population is exposed to an average acrolein concentration of 1.3 μg/m^3 with a median value of 0.6 μg/m^3. The ATSDR (2007) determined that, based on the mean estimate for acrolein concentration derived from the Canadian study (1.3 μg/m^3) and a standard inhalation volume of 20 m^3 of air per day, an average adult will inhale 26 μg acrolein/day.

Emissions and modeled acrolein concentrations were queried from the USEPA National-Scale Air Toxics Assessment http://www.epa.gov/ttn/atw/natamain/index.html (NATA; USEPA, 2013D). NATA is EPA's ongoing comprehensive evaluation of air toxics in the United States. The USEPA developed NATA as a state-of-the-science screening tool for state/local/tribal agencies to prioritize pollutants, emission sources, and locations of interest for further study in order to gain a better understanding of risks. NATA assessments do not incorporate refined information about emission sources, but rather, use general information about sources to develop estimates of risks which are more likely to overestimate impacts than underestimate them. The resulting risk estimates are purposefully more likely to be overestimates of health impacts than underestimates, and thus they are health protective. FDEP downloaded the most recent NATA results (USEPA, 2005A). Data for all Florida counties were queried from the database: http://www.epa.gov/ttn/atw/nata2005/tables.html. The estimated total statewide atmospheric acrolein concentration was 0.06755031307 μg/m^3 from point and non-point sources.

For the purpose of retaining consistency in calculating exposure for RSC determination the inhalation rate of 16 m^3/day (USEPA, 2011A) and a standard body weight of 70 kg (USEPA, 1997) were utilized in the exposure calculation. The average acrolein-based air concentration utilized to estimate average daily exposure was 0.20 μg/m^3 due to the fact that it represents the most conservative estimate located within the United States. The resultant estimated average daily dose of acrolein received through inhalation was 4.5 x10^{-5} mg/kg-day.

<u>Soil</u>

Acrolein volatilizes from soil (half-life of 7.5 – 10.2 hours) and is easily metabolized within soil, being mineralized to carbon dioxide. Microbes also contribute to acrolein's degradation (HSDB, No. 177). Data and information associated with typical concentrations of acrolein in soils could not be located. It is estimated that exposure to acrolein though soil ingestion is minimal if not negligible due to the volatility of acrolein.

<u>Treated drinking water</u>

Acrolein has not been detected in drinking water (IPCS, 1992). Concentrations of acrolein in treated drinking water supplies could not be located. It is estimated that exposure to acrolein through treated drinking water ingestion is minimal if not negligible due to the volatility of acrolein. According to USEPA (2008B), acrolein would likely volatilize before and during the aeration stages of drinking water treatment.

Oceanic/marine concentrations

Information and data concerning typical acrolein concentrations detected in oceanic/marine environments could not be located.

Diet (other than fresh or estuarine fish)

Acrolein is present in a variety of foodstuffs. It occurs naturally in the human body in small quantities as a metabolic byproduct. Assessing acrolein exposure through diet, however, is complicated by analytical difficulties and the lack of reliable content measurements (Abraham *et al.* 2011). According to Stevens and Maier (2008), acrolein is ubiquitously detected in cooked foods due to the fact that acrolein is inherently formed from carbohydrates, vegetable oils, animal fats, and amino acids during the process of heating. Various sources report a wide range of acrolein concentrations in different food types. The IARC (1995), the ATSDR (2007), and the IPCS (2002) report acrolein concentrations for various fruits, vegetables, meats, cheeses, food items cooked in oil/fats at different temperatures, alcohol, tea, and coffee. According to the IPCS (2002), the concentration of acrolein detected in food is typically <40 µg/g and in most instances is <1 µg/g. For example, the IARC (1995) reported that acrolein has been detected in cheeses at concentrations ranging from 290-1300 ppb (µg/kg) and the ATSDR (2007) reported acrolein has been detected at concentrations ranging from <0.01–0.05 ppm in various fruits and up to 0.59 ppm in cabbage, carrots, potatoes, and tomatoes. As reported by the IPCS (2002), research conducted by Robles (1968) and Zitting & Heinonen (1980) has found that acrolein is also produced as a thermal degradation product of cellophane and polystyrene thermoplastics used to package foods although data on the extent of migration to packaged food items have not been identified. Even though acrolein is detected in a large variety of different food types and is considered ubiquitous in cooked foods not enough data could be located to quantify a reliable holistic acrolein-based dietary exposure estimate that the general population would be exposed to when consuming a typical diet.

Ambient exposure sources

Acrolein is produced naturally by fermentation processes, as a volatile component of oils within oak trees, in biogenic emissions from pine and deciduous forests, as a product of incomplete combustion of organic matter (e.g., forest fires), and by the photochemical oxidation of hydrocarbons in the atmosphere (Ciccioli *et al.,* 1993; USEPA, 2009A).

Acrolein volatilizes from surface waters fairly rapidly (half-life, 23 hours from a model river that is one meter deep) (ATSDR, 2007). Consequently, bioaccumulation is not expected to significantly occur (IPCS, 1992; IPCS, 2002; HSDB, No. 177). The estimated bioconcentration factor of 3 (USEPA, 2003) lends further support to a lack of potential for bioconcentration in aquatic organisms.

Furthermore, comparing various measured and estimated BCF values, acrolein does not bioaccumulate significantly in fish (Bysshe, 1982; Hansch and Leo, 1995; Veith *et al.,* 1980).

RSC Calculation

The exposure estimates described above were used to estimate total non-surface water exposure as summarized below in **Table 1**.

Table 1. Estimated average daily acrolein exposure received through non-ambient sources by the general population.

Exposure Route	Estimated Exposure (mg/kg bw-d)
Inhalation of air	4.5×10^{-5}
Soil ingestion	Negligible
Treated drinking water ingestion	Negligible
Diet	Unable to quantify
Estimated total daily dose	**Insufficient information**

The oral Rfd for acrolein is 5×10^{-4} mg/kg-day (USEPA, 2013C). The inhalation exposure route represents 9% of the acrolein reference dose. Inhalation represents one of the main routes of acrolein exposure an individual may encounter due to the volatile nature of this chemical. It is clear that individuals can also be potentially exposed to acrolein through diet given its ubiquitous existence in cooked foods, detected existence in different types of raw (uncooked) foods and beverages, and potential existence in certain types of food packaging. However, data were lacking to quantify a holistic dietary exposure. Therefore, due to the fact that there is evidence that the general public is exposed to acrolein through sources other than ambient sources (*e.g*., surface waters, freshwater/estuarine fish consumption) and evidence suggesting a lack of significant bioaccumulation in aquatic biota an RSC of 0.2 (EPA floor) was used for acrolein due to information adequacy considerations.

Bis (2-chloroisopropyl) Ether (BCPE)

Background

Bis (2-chloroisopropyl) ether (CASRN 108-60-1) has several synonyms, including BCPE, bis (2-chloro-1-methylethyl) ether, dichlorodiisopropyl ether, dichloroisopropyl ether, 2,2'-oxybis(2-chloropropane), BCMEE, and a number of other names (USEPA, 2013C). For the purposes of this summary, the abbreviation BCPE will be used. BCPE is used in a variety of manufacturing processes and products, including paint and varnish removers, spotting agents, cleaning solutions, dyes, resins, and pharmaceuticals. As an additive to certain soap solutions, it is used in cleaning textiles. It is also an important by-product in the manufacture of propylene oxide and propylene glycol

(NTP, 1982). BCPE has been found in industrial plant effluents and in tap water, particularly those with intakes below dischargers.

BCPE releases to air exist as vapor concentrations, degrading in the presence of photochemically-produced hydroxyl radicals with an estimated half-life of 28 hours. BCPE is expected to be highly mobile in soils and may be resistant to biodegradation (NCBI, 2013B). Volatilization from moist soils and water is an important fate process. The volatilization half-life of BCPE is estimated at 19 hours (river model) and 10 days (lake model) (NCBI, 2013B). However, other sources note that BCPE will hydrolyze rapidly if released to water or moist soil with an estimated hydrolysis half-life of < 38.4 seconds in water, further noting that biodegradation, bioconcentration (in aquatic organisms), and adsorption to soil and sediment are not expected to be significant fate processes (Mabey *et al.,* 1982; HSDB, No. 503). It is predicted that the primary exposure routes to BCPE are through inhalation of contaminated air and ingestion of contaminated drinking water (NCBI, 2013A). Bioconcentration factors ranging from 5.2 to 12 suggest that bioconcentration in aquatic organisms is low (NCBI, 2013B).

Exposure Source Determinations

Manufacturing and release

According to the United States Environmental Protection Agency's Toxic Release Inventory (TRI) Explorer, total reported on-site disposal or other releases[29] of BCPE in 2011 accounted for 345 pounds with the majority of release/disposal occurring through fugitive air emissions and surface water discharges (TRI2011, 2013A). Total reported off-site disposal or other releases[30] in 2011 accounted for zero pounds of BCPE (TRI2011, 2013A). The total reported on- and off-site disposal or other releases for BCPE in 2011 was 345 pounds (TRI2011, 2013A). Total reported on-site disposal or other releases in 2012 accounted for 101.9 pounds of BCPE with the majority of disposal/release occurring through fugitive air emissions (TRI2012, 2013B). Total reported off-site disposal or other releases in 2012 accounted for zero pounds of BCPE (TRI2012, 2013B). The total

[29] Total reported on-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other on-site landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), fugitive air emissions, point source air emissions, surface water discharges, underground injection Class II-V wells, land treatment, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), and other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R).

[30] Total reported off-site disposal or other releases associated with TRI data include: underground injection to Class I wells, RCRA Subtitle C landfills, other landfills (those not authorized under Subtitle C of RCRA to accept hazardous wastes), storage only, solidification/stabilization (metals only), wastewater treatment (metals only), POTWs (metal and metal compounds), underground injection Class II- V wells, RCRA Subtitle C surface impoundments, other surface impoundments (those not authorized under RCRA to accept hazardous waste for disposal), land treatment, other land disposal (disposal to land that does not fall into one of the other on-site land release categories found in section 5.5.1 through 5.5.3 on the TRI From R), other off-site management (chemicals in waste managed by techniques not specifically listed in section 6.2 of TRI Form R), waste broker, and unknown.

reported on- and off-site disposal or other releases for BCPE in 2012 was 101.9 pounds (TRI2012, 2013B). Information/data retrieved from the USEPA's TRI explorer tool does not represent an exhaustive list of disposals/releases of chemicals due to the fact that only certain types of facilities are required to report this type of information.

Non-ambient Exposure Sources

Treated drinking water

Information and data concerning concentrations of bis (2-chloroisopropyl) ether detected in drinking water is scarce. In 1976 the United States Environmental Protection Agency conducted Phase II of its National Organic Monitoring Survey, an initiative to analyze drinking water in the United States for detections of specific chemicals. Data from this study was published by the U.S. EPA in the 1980 Ambient Water Quality Criteria Document for Chloroalkyl Ethers. From this study, BCPE was detected in the finished (treated) drinking water of 8 cities out of the 113 cities under study. The mean BCPE concentration generated from the 8 positively detect sites was 0.17 µg/L, which indicated a 7.1% incidence among cities surveyed (USEPA, 1980A). The Ambient Water Quality Criteria Document for Chloroalkyl Ethers also reported a variety of BCPE concentrations detected in additional finished drinking water samples from facilities around the United States. For example, BCPE was detected in finished drinking water samples at a concentration of 0.8 µg/L in Evansville, Indiana and in finished drinking water samples at the Carrollton Station and two facilities in Jefferson Parish, Louisiana at concentrations of 0.18, 0.08, and 0.03 µg/L, respectively (USEPA, 1980A). According to the Hazardous Substance Data Bank (HSDB; No. 503), BCPE has also been detected in drinking water in New Orleans, Louisiana at an average concentration of 0.10 ng/m^3. Although various concentration of BCPE has been detected in treated drinking water, information on drinking water is too limited to confidently estimate an exposure for the general population.

Air

Information and/or data could not be located concerning typical bis (2-chloroisopropyl) ether concentrations in ambient air.

Soil/sediments

Information and/or data could not be located concerning bis (2-chloroisopropyl) ether concentrations detected in typical soils. However, according to an analysis of STORET data conducted by staples *et al.* (1985), BCPE has been detected in sediments at a median concentration of < 500 µg/kg.

Diet

Information and/or data could not be located concerning bis (2-chloroisopropyl) ether concentrations detected in different food types or average dietary exposure measurements associated with bis (2-chloroisopropyl) ether.

Ambient Exposure Sources

BCPE has been found in rivers as a result of industrial discharges from propylene glycol production in amounts ranging from 0.2 to 5 µg/L (HSDB, No. 503). According to Staples *et al.*'s (1985) analysis of STORET data, BCPE has been detected in ambient surface waters at a median concentration of < 10 µg/L (Staples *et al.,* 1985). In addition, BCPE has been detected in ambient waters at mean concentrations of 0.10 µg/L in the New Orleans/Baton Rouge, Louisiana area and 19 µg/L in the Houston, TX area (HSDB, No. 503). It is predicted that BCPE will not significantly bioaccumulate in aquatic biota due to its low BCF.

RSC Calculation

The exposure estimates described above were used to estimate a total non-surface water exposure as summarized below in **Table 1**.

Table 1. Estimated average daily bis (2-chloroisopropyl) ether exposure received through non-ambient sources by the general population.

Exposure Route	**Estimated Exposure (mg/kg bw-day)**
Inhalation of Air	No information located
Soil ingestion	No information located
Treated drinking water ingestion	Limited information
Diet	No information located
Estimated total daily dose	**Insufficient information**

The oral RfD for bis (2-chloroisopropyl) ether is 0.04 mg/kg-day (USEPA, 2013C). Exposure and contamination level data are lacking for the exposure routes of interest needed to calculate a chemical-specific RSC for this chemical. Therefore, an RSC of 0.2 (EPA floor) was used for bis (2-chloroisopropyl) ether due information adequacy considerations.

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ATTACHMENT E

A Preliminary Evaluation of the Application of USEPA's National Bioaccumulation Methodology in the Derivation of Human Health-Based Surface Water Quality Criteria for Florida

ARCADIS Design & Consultancy for natural and built assets

Florida Pulp & Paper Association
Environmental Affairs

A Preliminary Evaluation of the Application of USEPA's National Bioaccumulation Methodology in the Derivation of Human Health-Based Surface Water Quality Criteria for Florida

July 21, 2016

EVALUATION OF BAF METHODOLOGY

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CONTENTS

TABLES

ACRONYMS AND ABBREVIATIONS

AWQC	ambient water quality criteria
BAF	bioaccumulation factor
BaP	benzo(a)pyrene
BCF	bioconcentration factor
BSAF	biota-sediment accumulation factor
Cwfd	concentration of chemical freely dissolved in the water column
DOC	dissolved organic carbon
DOM	dissolved organic matter
FCM	food chain multiplier
FDEP	Florida Department of Environmental Protection
f_{fd}	fraction of total concentration freely dissolved
f_l	fraction of tissue that is lipid
HHC	human health-based criteria
HHWQC	Human Health Water Quality Criteria
Π_{socw}	sediment-water concentration quotient
k_d	dietary uptake rate constant
k_m	metabolic transformation rate constant
K_{ow}	n-octanol-water partition coefficient
PAH	polycyclic aromatic hydrocarbon
PCB	polychlorinated biphenyls
POC	particulate organic carbon
SWQC	surface water quality criterion
TL	trophic level
USEPA	United States Environmental Protection Agency

EXECUTIVE SUMMARY

This white paper presents preliminary findings of a review and evaluation of the methods used by the Florida Department of Environmental Protection (FDEP) to estimate bioaccumulation of compounds from Florida surface waters into fish and shellfish consumed by Floridians. The estimation of such bioaccumulation is a key component in developing the human health-based surface water quality criteria (HHC) proposed by FDEP in May 2016. FDEP relied primarily, with exceptions noted in the white paper, on the methods and models developed and used by United States Environmental Protection Agency (USEPA) to derive the national 2015 Human Health Water Quality Criteria (HHWQC).

It is important to understand that USEPA has an expressed preference for developing HHC based on bioaccumulation factors (BAFs) rather than bioconcentration factors (BCFs) because BAFs account for exposure of fish and shellfish from all exposure pathways (e.g., water, diet, sediment) while BCFs account for exposure from only water. When measured BAFs are available USEPA's procedure uses those to estimate bioaccumulation. When measured BAFs are not available USEPA estimates BAFs by multiplying either measured or modeled BCFs by a food chain multiplier (FCM). The FCM is intended to account for exposure of fish and shellfish from the non-water exposure pathways.

This white paper focuses on two aspects of USEPA's procedure as it was used by FDEP. The first is the process and data used to develop measured BCFs for compounds that do not have field measured BAFs. This white paper uses an example compound and focuses on the process and data used to estimate the BCF for benzo(a)pyrene (BaP) a polycyclic aromatic hydrocarbon (PAH) that is used as a surrogate by USEPA and FDEP to estimate the bioaccumulation of six other PAHs. The second aspect of USEPA's process addressed in this white paper is the applicability of national FCMs to surface waters in Florida. The FCMs used by USEPA (and FDEP) are based on a model developed to estimate bioaccumulation of compounds in a food web representative of the Great Lakes. This white paper examines some of the assumptions used by USEPA to characterize surface water and food webs in the Great Lakes and compares them to surface waters and food webs in Florida to determine the applicability of the FCMs to Florida surface waters.

Review of the approach used by USEPA (and FDEP) to develop the BAF for BaP identified three key concerns that affect the final BAF (or in the case of FDEP, the BCF) used to derive the proposed HHC.

- The USEPA database includes three invertebrate species that are not representative of shellfish consumed by Floridians (i.e., the water flea (*Daphnia magna*), an amphipod (*Pontoporeia hoyi)*, and a mayfly (*Hexagenia limbata*). Whether the accumulation of BaP in typically consumed shellfish is well represented by BCFs from amphipods, mayflies and water fleas is unknown. What is known is that these three organisms are very different from those that are regularly consumed. Until it has been shown that their BCFs are representative of regularly consumed species, it might be best to exclude them when estimating the BCFs of regularly consumed shellfish species. Excluding these three species causes the final BCF for BaP to increase.
- USEPA's (and FDEP's) BAF derivation process includes establishing something USEPA refers to as a baseline BAF. A baseline BAF is expressed on a 100% lipid basis and assumes that all of a compound is dissolved in water (i.e., none of the compound in the water column is bound to organic carbon, so all of the compound is available to be accumulated). Most studies reporting

BCFs do not provide information on the fraction of BaP dissolved in the water column versus the fraction sorbed to organic carbon suspended in the water column. To estimate the fraction of BaP dissolved in the water column USEPA needed to make assumptions about how much organic carbon was present in the experiments reporting BCFs. USEPA assumed all of those experiments had organic carbon equal to the median measured in U.S. surface waters. However two thirds of the BaP BCF studies used filtered water. Such water will likely have a much lower organic carbon concentration than that assumed by USEPA. When an organic carbon concentration more representative of filtered water is used to derive baseline BAFs, the baseline BAF for BaP decreases by about 40%.

- For compounds that do not have measured BAFs, a key step of USEPA's process for deriving a baseline BAF is multiplying a BCF by a FCM. USEPA's guidance lists certain characteristics of a compound that preclude the application of a FCM. One of those characteristics is "high metabolism" which is how USEPA classified BaP. Thus, USEPA should not have multiplied the BaP BCFs by FCMs to derive a baseline BAF. FDEP recognized this incorrect application of a FCM and did not apply a FCM to the BCF of BaP when developing the proposed HHC. The effect of not including the FCM is substantial, baseline BAFs decrease by several-fold.

When all of the above factors are accounted for, the Florida-specific BAF for BaP becomes 484 kilograms per liter (L/kg); lower than the BAF of 600 L/kg used by FDEP in the proposed HHC and lower than USEPA's national BAF for BaP of 3,900 L/kg.

Review of the applicability of national FCMs to Florida surface waters and food webs revealed numerous reasons to believe the national default assumptions used by USEPA to derive national FCMs are unlikely to be representative of Florida conditions.

- The model used by USEPA to derived national FCMs is based on and calibrated for a Great Lakes food web using PCB data. A Florida based food web will have substantially different inputs and structure and could result in a very different FCMs. For example Florida waters do not support alewives, smelt or salmonids and the lipid content of many fresh water species appears to be lower in Florida than in the Great Lakes. At this point it is unknown whether food webs more representative of Florida surface waters will have higher or lower FCMs than those derived for the Great Lakes but the components and structure will clearly be very different.
- USEPA's model assumes that surface waters have had a long history of loading of compounds followed by a relatively recent reduction in such loading (such as PCBs in the Great Lakes and Hudson River in the 1980's and 1990's). That scenario of high historic loading leads to a high proportion of a compound in sediments compared to conditions closer to equilibrium. The effect of that high proportion of a compound in sediments is to increase FCMs. FCMs decrease substantially when compound loadings expected to be representative of most waters in the U.S. and Florida are employed in the FCM model.
- The FCMs developed by USEPA assume no metabolic transformation of a compound by fish and shellfish. Yet USEPA (and FDEP) are using the FCMs developed using the assumption of no metabolic transformation to derive HHC for many compounds that are likely to be metabolized to some degree by fish or shellfish or both. The potential effect on FCMs of incorporating metabolism was investigated for pentachlorophenol, heptachlor, and 1,3-dichlorobenzene. When

the compound-specific metabolic transformation rate constants were incorporated into the FCM model, the FCMs dropped substantially for all three chemicals.

- Finally, the temperature used in the USEPA model is much cooler than might be expected in Florida waters. Use of a higher temperature in the FCM model increases FCMs because the higher temperature results in an increase in dietary intake in the model. Because the model assumes no metabolic transformation, the increased dietary intake is not balanced by what one might expect to be an increased rate of metabolic transformation as temperature increases.

In summary, the preliminary evaluations presented in this white paper provide several lines of strong evidence that the application of USEPA's national BAF procedure to estimate bioaccumulation in Florida surface waters is premature and does not represent good science. Additional evaluation is necessary to identify those aspects of USEPA's national BAF methodology that are applicable to Florida and those that need Florida-specific modification before they can be used to derive human health-based criteria for Florida surface waters. While the preliminary evaluation of some of the individual parameters of the FCM model suggest that BAFs in Florida may be lower than estimated by USEPA for the Great Lakes, the combined effect of all such modifications, and whether those will lead to higher or lower estimates of bioaccumulation, is unknown at this time.

Introduction

To estimate the bioaccumulation of substances from surface water into fish and shellfish the Florida Department of Environmental Protection (FDEP) relied primarily, with exceptions as noted below, on the methods and models developed and used by United States Environmental Protection Agency (USEPA) to derive the national 2015 Human Health Water Quality Criteria (HHWQC) and as further explained by USEPA in their January 2016 supplemental information for development of national bioaccumulation factors (USEPA 2016). See Table 1 for a comparison of Florida and National bioaccumulation factors (BAFs).

USEPA's process has an expressed preference for basing HHWQC on BAFs rather than bioconcentration factors (BCFs) because BAFs account for exposure of fish and shellfish from all exposure pathways (e.g., water, diet, sediment) while BCFs account for exposure from only water. When measured BAFs are available USEPA's procedure uses those to estimate bioaccumulation. When measured BAFs are not available USEPA estimates BAFs by multiplying either measured or modeled BCFs by a food chain multiplier (FCM). The FCM is intended to account for exposure of fish and shellfish from the non-water exposure pathways. Exceptions to this process include inorganic compounds that are not expected to biomagnify, ionized organic compounds, organic compounds with log K_{ow} of less than 4, and organic compounds that are highly metabolized. For compounds that fall into either of these four categories USEPA's procedure suggests using a field measured BAF and if such is not available, a laboratory derived BCF.

This white paper focuses on two aspects of USEPA's procedure as it was used by FDEP to estimate bioaccumulation of substances from Florida surface waters into fish and shellfish. The first is the process and data used to develop measured BCFs for compounds that do not have field measured BAFs. Measured BCFs are used to estimate accumulation of 20 of 88 compounds for which revised HHC are proposed. This white paper focuses on the process and data used to estimate the BCF for benzo(a)pyrene (BaP) a polycyclic aromatic hydrocarbon (PAH) that is used as a surrogate to estimate the bioaccumulation of six other PAHs (benzo(a)anthracene, benzo(b)fluoranthene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, indeno(1,2,3-cd) pyrene). Whether the comments presented below for the derivation of the BCF for BaP apply to all the other compounds for which measured BCFs are used is not known; what is known is that they do apply to a total of seven PAHs, which represents slightly more than a third of the compounds for which measured BCFs were used.

The second aspect of USEPA's process to estimate bioaccumulation that is addressed in this white paper is the applicability of the FCMs to surface waters in Florida. A FCM is used by FDEP to estimate the accumulation of 60 of 88 compounds for which revised HHWQC are proposed. The FCMs used by USEPA (and FDEP) to adjust BCFs to account for exposures other than water, are based on a model adopted by USEPA in 1993 (Gobas 1993). That model was developed to estimate bioaccumulation of compounds such as polychlorinated biphenyls (PCBs) in a food web representative of the Great Lakes. This white paper examines some of the assumptions used by USEPA to characterize surface water and food webs in the Great Lakes and compares them to surface waters and food webs in Florida to determine the applicability of the FCMs to Florida surface waters. For some model parameters, the white paper also presents a sensitivity analysis demonstrating whether FCMs specific to Florida surface waters

would be different (either higher or lower) from Great Lakes-based FCMs. The sensitivity analysis does not address all parameters used in the Great Lakes FCM model. Thus, it remains unknown whether FCMs based on a model that truly represents Florida surface waters and food webs, would be higher or lower than the FMCs used to derive the currently proposed HHWQC.

Background: Derivation of Surface Water Quality Criteria for Protection of Human Health

FDEP used USEPA guidance (USEPA 2000) to derive surface water quality criteria (FDEP 2016). The equation for non-carcinogenic compounds for consumption of water and organisms is as follows:

$$SWQC(\mu g/L) = \frac{\left[RfD\left(^{mg}/_{kg \cdot d}\right) x\, RSC\right] \times BW\,(kg) \times 1{,}000\,(\mu g/mg)}{DI\,(L/d) + \Sigma_{i=2}^{4}\left[FCR_i\left(^{kg}/_{d}\right) \times BAF_i\left(^{L}/_{kg}\right)\right]}$$

Where:

SWQC = surface water quality criterion (µg/L);

RfD = compound-specific reference dose (mg/kg-d);

RSC = Relative source contribution factor to account for non-water sources of exposure (not used for linear carcinogens);

BW = body weight (kg);

DI = drinking water intake (L/d);

FCR_i = fish consumption rate for aquatic trophic levels (TLs) 2, 3, and 4 (kg/day);

BAF_i = bioaccumulation factor for aquatic TLs 2, 3, and 4 (L/kg); and

$\Sigma^4_{i=2}$ = summation of values for aquatic TLs, where the letter i stands for the TLs to be considered, starting with TL2 and proceeding to TL4.

For carcinogenic compounds, the reference dose term in the denominator is replaced by [Target Risk/CSF (mg/kg-d)] where:

CSF = Cancer slope factor (mg/kg-d); and

Target Risk = Allowable incremental life-time increased cancer risk (usually either $1x10^{-6}$ of $1x10^{-5}$).

For SWQC developed to protect human health from exposures associated with consumption of organisms only, the drinking water intake term is removed from the equation.

FDEP used a probabilistic approach (Monte Carlo simulation) to solve these equations and calculate HHC[1]. This was accomplished by specifying a distribution for some of the parameters (e.g. body weight, fish consumption rate, drinking water rate) rather than using a point estimate for that parameter, randomly choosing from that distribution and solving the equation in multiple iterations to ensure that specific segments of the population are protected at specified target risk levels. Other parameters were characterized using point estimates (e.g. bioaccumulation factors, reference doses, cancer slope factors, relative source contribution (RSC)). The general categories of parameters are summarized briefly below.

Toxicity Parameters – FDEP used values from the IRIS database and alternative sources for reference doses and cancer slope factors similar to the approach used by USEPA in the calculation of their 2015 HHWQC. These were entered as point estimates in the equations. FDEP used a default value of 0.2 for the RSC.

Exposure Parameters – FDEP developed state specific probability distributions for exposure parameters for the probabilistic approach. The distributions for drinking water intake and body weight are based on national recommendations from the 2011 USEPA Exposure Factors Handbook. The fish consumption rate (FCR) distribution is based on USEPA's 2014 Estimated Fish Consumption Rates for the U.S. Population and Selected Subpopulations. FDEP created FCR distributions for the probabilistic analysis based on the geographic regions representative of Florida, Atlantic Coast, Gulf Coast, and Inland South.

Bioaccumulation Parameters – In general, FDEP's approach followed the methodology described by USEPA (2003) but used Florida-specific values for lipid content of fish species and organic carbon content in surface waters. Other critical parameters used in the BAF calculations, particularly food chain multipliers (FCMs), were not Florida-specific and were based on the national default values. The final calculated BAFs were entered as point estimates in the HHC equations. A detailed analysis of the methodology used by FDEP to calculate BAFs is described below and includes a comparison of Florida-specific and National BAFs.

FDEP's Derivation of BCFs and BAFs for Florida Surface Waters

In general FDEP followed the USEPA methodology to derive BCFs/BAFs for use in WQC calculations (USEPA, 2000, 2003, 2016) and used the same methods and the same studies to derive BCFs/BAFs as USEPA. For most compounds[2] the methodology involves estimating a baseline BAF (i.e. a BAF based on the dissolved fraction and adjusted for lipid concentration) based on field or laboratory studies if available. If field or laboratory studies are not available, the baseline BAF is estimated from a compound's n-octanol-water partition coefficient. The baseline BAFs are averaged by species and trophic level (geometric mean) and a food chain multiplier (FCM) is applied to each trophic level for chemicals classified as non-metabolized. With the exception of PAHs, FDEP used the baseline BAFs provided in the supplemental information provided by USEPA (USEPA, 2016). The baseline BAFs were then converted to Florida BAFs using state specific assumptions about the concentration of dissolved organic carbon (DOC) and particulate organic carbon (POC) is surface water, parameters used to calculate the freely

[1] The May 2016 FDEP technical support document refers to the proposed criteria as HHC. These are the same as the SWQC referred to in the formula above. USEPA refers to such criteria as ambient water quality criteria (AWQC). Such criteria have also been referred to as HHWQC. Depending upon citation, all of these terms may appear in this white paper and refer to surface water quality criteria for protection of human health.
[2] BCFs and not BAFs were developed and used to derive the proposed HHC for some compounds.

dissolved fraction in Florida waters, and Florida-specific assumptions for the lipid content in each trophic level. FDEP assumed lipid contents of 1.8%, 1.5% and 2% for TL2, TL3 and TL4 respectively. For PAHs, FDEP determined that USEPA (2015a) failed to correctly account for high metabolic transformation rates. Specifically, USEPA calculated the BAFs for 12 PAHs by multiplying laboratory BCFs by FCMs. FDEP noted that this is not consistent with USEPA guidance for highly metabolized compounds and therefore they recalculated the baseline BAFs for 12 PAHs based on the laboratory BCF results provided by USEPA (2016) but without applying FCMs. There was another inconsistency with guidance on the part of USEPA's baseline BAF calculations. Baseline BAFs are supposed to be calculated based on the study specific measurements of the freely dissolved fraction of a chemical during the experiment. However, USEPA used default values of DOC and POC to calculate baseline BAFs from field or laboratory based BAFs or BCFs. FDEP did not recognize this departure from guidance in USEPA's calculations and used the baseline BAFs as presented in the supplemental material (USEPA 2016). A discussion of the potential implications of this departure from guidance is further discussed below.

The USEPA methodology prescribes four methods for deriving BAFs presented below in order of preference given the amount of available information from literature.

1. Measured BAFs derived from data obtained from a field study (i.e., field measured BAFs).
2. BAFs predicted from biota-sediment accumulation factors (BSAFs) obtained from a field study (i.e., field-measured BSAFs).
3. BAFs predicted from laboratory-measured BCFs, with or without adjustment by a FCM.
4. BAFs predicted from a compound's n-octanol-water partition coefficient (K_{ow}), with or without adjustment by a FCM.

The methods are to be chosen preferentially in the order shown depending on the amount of information available in the literature and based on the properties of the compound and whether or not the compound is metabolized as shown in the flow chart below. BAFs and BCF were not combined in calculations. Each method results in an estimate of a baseline BAF for each trophic level using one of the following equations:

$$(\text{Baseline BAF})_{TL\ n} = [BAF_T^t/f_{fd} - 1] \bullet 1/f_l$$

$$(\text{Baseline BAF})_{TL\ n} = (FCM)_{TL\ n} \bullet [BCF_T^t/f_{fd} - 1] \bullet 1/f_l$$

$$(\text{Baseline BAF})_{TL\ n} = K_{ow} \bullet (FCM)_{TL\ n}$$

Where:

$(\text{Baseline BAF})_{TL\ n}$ = baseline BAF for TL "n" (L/kg-lipid);

BAF_T^t = total BAF from field sample (i.e., total concentration of chemical in tissue / total concentration of chemical in water [L/kg-tissue]);

BCF_T^t = total BCF from laboratory measure (i.e., total concentration of chemical)

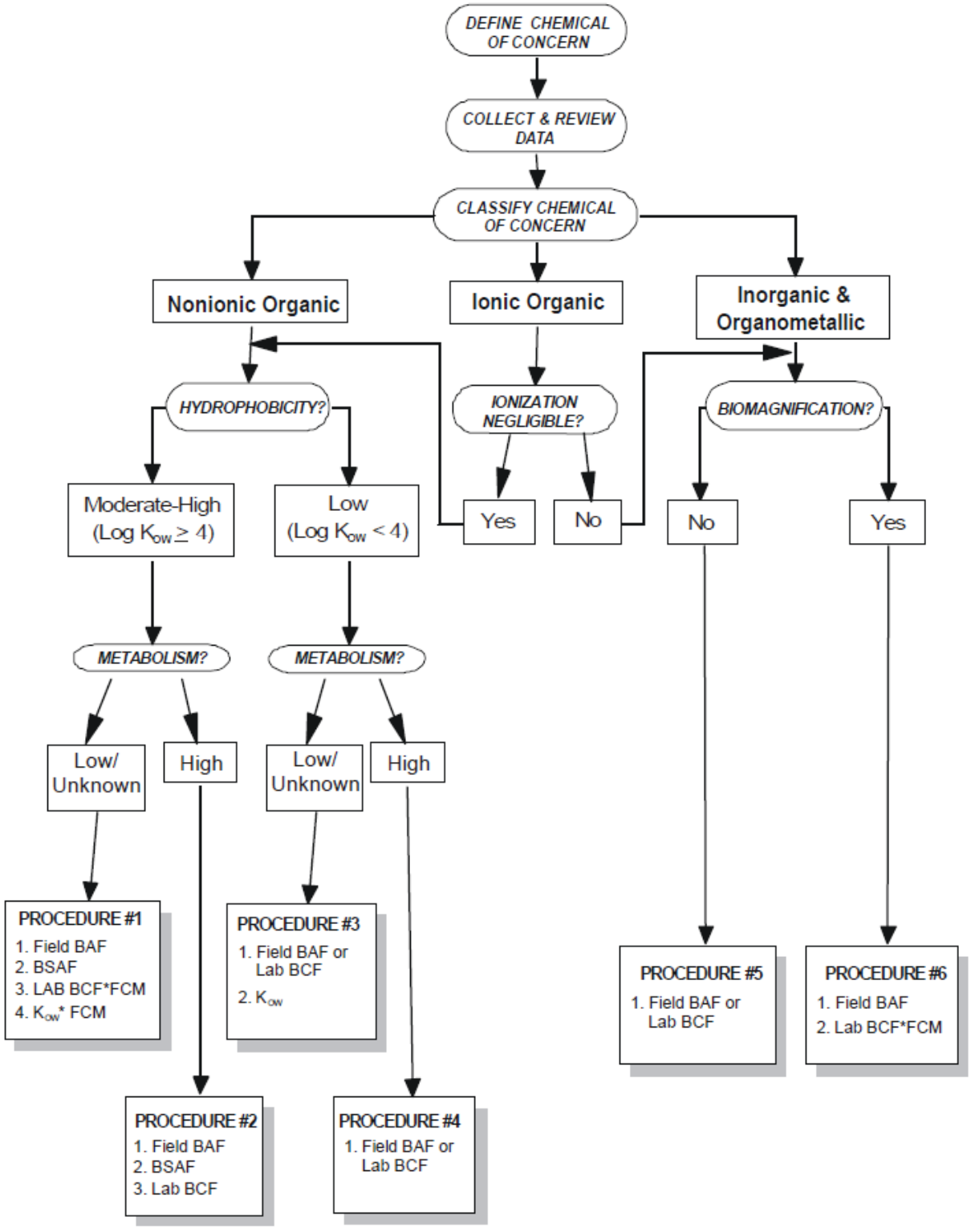
in tissue / total concentration of chemical in water [L/kg-tissue]);

f_{fd} = fraction of the total concentration of chemical in water that is freely dissolved (in field or laboratory sample);

f_l = fraction of tissue that is lipid (in tested species);

FCM = FCM for TL “n”; and

K_{ow} = n-octanol-water partition coefficient.


DEFINE CHEMICAL OF CONCERN
COLLECT & REVIEW DATA
CLASSIFY CHEMICAL OF CONCERN
Nonionic Organic
Ionic Organic
Inorganic & Organometallic
HYDROPHOBICITY?
IONIZATION NEGLIGIBLE?
BIOMAGNIFICATION?
Moderate-High (Log Kow ≥ 4)
Low (Log Kow < 4)
Yes
No
No
Yes
METABOLISM?
METABOLISM?
Low/ Unknown
High
Low/ Unknown
High
PROCEDURE #1
1. Field BAF
2. BSAF
3. LAB BCF*FCM
4. Kow* FCM
PROCEDURE #3
1. Field BAF or Lab BCF
2. Kow
PROCEDURE #5
1. Field BAF or Lab BCF
PROCEDURE #6
1. Field BAF
2. Lab BCF*FCM
PROCEDURE #2
1. Field BAF
2. BSAF
3. Lab BCF
PROCEDURE #4
1. Field BAF or Lab BCF

For compounds that fall under procedures #1 and #6 and when the log K_{ow} is greater than or equal to 4, the species is assigned to a particular TL (i.e., 2, 3, or 4) and an FCM is applied. For other cases, the FCM is dropped from the equation (or equivalently set to 1.0). FCMs were developed by USEPA using a food web model further described below. FDEP applied the USEPA-derived FCMs where appropriate to calculate baseline BAFs (i.e. all baseline BAFs used by FDEP are the same as USEPA baseline BAFs with the exception of the 12 PAHs mentioned above).

Multiple baseline BAFs, either from laboratory or field studies (but not both), are averaged by species and then by trophic level using the geometric mean to calculate a final baseline BAF for each TL. For study-based baseline BCFs/BAFs, estimates of f_{fd} and f_l are supposed to be study specific. However, in the Excel spreadsheet provided by USEPA as part of the supplemental information, it is clear that USEPA did not enter f_{fd} from the specific studies but rather estimated it using the national default values for DOC and POC and the following equation:

$$F_{fd} = 1 / [1 + POC \bullet K_{ow} + DOC \bullet 0.08 \bullet K_{ow}]$$

This departure by USEPA from their own guidance calls into question the validity of all the study-based baseline BAFs. Potential implications of this departure from guidance are further discussed below.

The final Florida BAFs were calculated in the same way as national BAFs except with Florida specific assumptions as follows:

$$\text{Florida BAF} = [(\text{Final Baseline BAF})_{TL\ n} \bullet (f_l)_{TL\ n} + 1] \bullet (f_{fd})$$

Where:

Florida BAF = final Florida BAF (L/kg-tissue);

Final Baseline $BAF_{TL\ n}$ = mean baseline BAF for TL “n” (L/kg-lipid);

$(f_l)_{TL\ n}$ = Florida specific estimate of lipid fraction at TL “n”, assumed to be 1.8%, 1.5% and 2.0% for TLs 2, 3, and 4, respectively, compared to the national lipid contents assumed by USEPA 1.9%. 2.6% and 3.0%, respectively; and

f_{fd} = fraction of total concentration freely dissolved based on Florida specific estimates of DOC and POC, assumed to be 12 mg/L and 0.6 mg/L, respectively, compared to the national concentrations assumed by USEPA of 2.9 mg/L and 0.5 mg/L, respectively.

Table 1 shows a comparison of the Florida derived BAFs and the USEPA derived national BAFs and which of the above four methods was used in the derivation. There are a total of 88 compounds for which Florida used BCFs/BAFs. The following methods were used: Log K_{ow}*FCM (n=54); Field BAFs (n=6); BCF*FCM, (n=3); Alternative BAF/(BCF*FCM)" (n=3); Alternative BAF (n=5); BCF (n = 12 PAHs); 1980 BCF for beryllium; and 2002 BCF (n=4). Alternative BAFs refer to a method of calculating one BAF to represent all three trophic levels. This is applied when data are not available to estimate BAFs for all 3 TLs. In general, FDEP used the same methods, field studies, and assumptions as USEPA. However, as noted above, unlike USEPA, FDEP did not apply FCMs when calculating baseline BAFs for 12 PAHs, ((Acenaphthene, Anthracene, Benzo (a) Anthracene, Benzo (a) Pyrene, Benzo (b) Fluoranthene, Benzo (k) Fluoranthene, Chrysene, Dibenzo (a,h) Anthracene, Fluoranthene, Fluorene, Indeno (1,2,3-cd) Pyrene, and Pyrene)). FDEP’s approach is correct because these compounds have been classified by USEPA as highly metabolized and, therefore, FCMs should not have been applied by USEPA.

For all other compounds FDEP used the same methodology as USEPA and for methods 1 through 3, FDEP used the same set of field BAFs or laboratory BCFs as USEPA to derive baseline. In these cases the differences between Florida BAFs and National BAFs are wholly attributable to the differences in Florida's assumptions for lipid content at each trophic level (which are lower than the national default assumptions) and their assumptions of POC and DOC of Florida surface waters (which are higher than the national default assumptions and result in lower estimates of the dissolved fraction). Florida's assumptions for both lipid and organic carbon concentration result in lower final BAF calculations as compared to national final BAFs. The degree of difference depends on hydrophobicity for organic compounds. Florida TL2 BAFs are about half as large as national BAFs when log K_{ow} > 6.5 but are not much different when log K_{ow} < 5.

Review of the Florida BAF for BaP

As noted above, this white paper focuses on the process and data used to estimate the BCF for BaP as an example of some of the short comings in that process and those data. Whether the shortcomings described below for the derivation the BCF for BaP apply to all the other compounds for which measured BCFs are used is not known. Arcadis has not review the underlying data and publications for the other compounds for which revised HHC are proposed. What is known is that the shortcomings do apply to a total of seven PAHs (BaP and the six PAH for which BaP is used as a surrogate (i.e., benzo(a)anthracene, benzo(b)fluoranthene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, indeno(1,2,3-cd) pyrene). These seven PAH represent slightly more than a third of the compounds for which measured BCFs were used.

The general process that USEPA followed to estimate a national BCF for a specific species from a specific study had four steps. FDEP adopted most of these steps when estimating accumulation of BaP in fish and shellfish (and the other six PAHs for which BaP is assumed to be a surrogate) with a very important exception. As a final step, USEPA multiplied the trophic level 2 and 3 BCFs for BaP by FCMs of 1 and 10.2, respectively to derive a BAF of 3900 for BaP even though USEPA classified BaP as having "high metabolism" (USEPA 2015). According to USEPA's supplemental information released in January 2016 (USEPA 2016), and consistent with the text describing the derivation of the BAF for BaP in USEPA (2015a), the BCF for BaP should not have been multiplied by a FCM because of the high metabolism classification. Use of FCMs is inappropriate for metabolized compounds because USEPA's FCM model assumed compounds are not metabolized[3]. Such an assumption does not apply to BaP or to the other PAHs. FDEP recognized this incorrect application of a FCM and did not apply a FCM to the BCF of BaP when developing the proposed HHC.

[3] According to USEPA (2016) other chemical characteristics also preclude the use of FCMs when using BCFs to derive baseline BAFs. One such characteristic is ionization. If a compound is expected to be ionized, an FCM should not be applied to a BCF to derive a baseline BAF. USEPA classified pentachlorophenol as an "ionic organic chemical, with ionization not negligible" (USEPA 2015b). Nevertheless, when deriving the baseline BAF for pentachlorophenol, and contrary to their guidance, USEPA used FCMs.

The first step in deriving a BCF for BaP was identifying and summarizing the BCFs reported in peer-reviewed literature for BaP[4]. At this point Arcadis has not conducted a comprehensive review of the available literature on BaP BCFs and, therefore, this white paper is not commenting on the completeness of the data set used by USEPA to derive the BCF for BaP. Other peer-reviewed studies reporting valid BCFs for BaP may be available. As part of the review of the peer-reviewed studies included in the USEPA database, Arcadis identified one study that reported a BCF that appears to have been entered incorrectly in the database. Jimenez et al. (1987) report a BCF of 608 L/kg but the database lists a BCF of 842 mg/L[5]. Arcadis was not able to identify an explanation for the discrepancies between the BCF reported by the study and the BCF listed in the database. The BCFs for BaP reported by the other studies agree with the database entries.

Of note regarding the 26 measured BCFs for BaP included in the database is a BCF for a water flea (*Daphnia magna*), a BCF for an amphipod (*Pontoporeia hoyi)*, which is close relative of beach lice, and a BCF for a mayfly (*Hexagenia limbata*). These species are used to estimate the accumulation of BaP into shellfish that Floridians regularly consume (e.g., crabs, shrimp, lobster, clams) but these species are very different from shellfish regularly consumed by Floridians. Whether the accumulation of BaP in typically consumed shellfish is well represented by BCFs from water fleas, amphipods and mayflies is unknown. What is known is that these three organisms are very different from those that are regularly consumed and until it has been shown that their BCFs are representative of regularly consumed species, it might be best to exclude them when estimating the BCFs of regularly consumed shellfish species. Other species for which BCFs are reported include three for Bluegill sunfish (*Lepomis marochirus*), one for shrimp (*Mysis relicta*), and 19 for zebra mussels (*Dreissena polymorpha).*

The second step in deriving a BCF for BaP is converting the BCFs reported for each species in each of the studies to what USEPA refers to as a baseline BAF[6]. The baseline BAF is expressed on a freely dissolved and 100% lipid basis. Some peer-reviewed studies report the lipid content of the species for which a BCF is presented, precluding the need to make assumptions about the lipid content of the test organisms. Other studies do not report the lipid contents and a default national species-specific lipid content (USEPA 2003) is used.

In almost all cases, the peer-reviewed study does not measure or estimate the freely dissolved concentration of a BaP in the setting from which the BCF was derived. The study simply reports the nominal concentration of BaP in the setting and reports the BCF on the basis of the nominal concentration. One exception to this is Landrum and Poore (1988). Landrum and Poore (1988) correct BaP uptake by mayflies for the fraction of the BaP that was bound to dissolved organic matter (DOM) in the test setting, recognizing that the increase in DOM can ultimately reduce the bioavailability of non-polar organics such as BaP measured in water. Thus, the BCFs for BaP reported by Landrum and Poore

[4] The database upon which USEPA and FDEP rely to develop BCFs/BAFs for BaP report both measured BCFs and measured BAFs from peer-reviewed literature for BaP. Because many more peer-reviewed BCFs are reported than are BAFs, USEPA relies on the reported BCFs and not the reported BAFs to derive a baseline BAF. Hence, the BaP example refers to peer-reviewed literature reporting BCFs.

[5] During Arcadis's review of the BaP dataset we also identified a discrepancy for one of the studies reporting a BAF for BaP. Frank et al. (1986) report a BAF of 676 mg/L, however a BAF of 3,236 mg/L is listed in USEPA's database.

[6] To be consistent with the terminology used by USEPA and FDEP this white paper uses the term "baseline BAF" when referring to either literature-derived BCFs or BAFs, even though in the case of BaP (and other chemicals as well) that baseline BAF is based on BCFs reported in the literature.

(1988) are expressed on based on a freely dissolved basis and, therefore, the fraction freely dissolved factor should not be applied. USEPA (and FDEP because they used the USEPA BCF) incorrectly applied a fraction freely dissolved correction factor to the BCF reported by Landrum and Poore (1998). The effect of removing the fraction freely dissolved correction factor of the BCF for BaP is discussed at the end of this section.

The freely dissolved fraction depends upon chemical-specific characteristics (log K_{ow}) as well as characteristics unique to the setting in which the BCF was measured (concentration of dissolved organic carbon (DOC) and particulate organic carbon (POC)). One can imagine that in a laboratory setting, using synthetic or filtered water, the amount of organic material in the water is much lower than it would be in a naturally occurring surface water. Additionally, and as USEPA (2000) states, POC is eliminated from the laboratory test water that is filtered prior to use in BCF and BAF experiments. Three of the five studies that report BaP BCFs used filtered lake waters: Gossiaux et al. (1996) and Landrum and Poore (1988) used water from Lake St. Clair, and Murray et al. (1991) used water collected from sites in Port Phillip Bay, Victoria , Australia. Assuming that the concentration of DOC in these filtered lake waters would be comparable to the national median DOC used by USEPA for all waters (i.e., 2.9 mg/L) does not seem unreasonable as the mean DOC concentration in lake waters was 2.9 mg/L as well (USEPA 2003). However, assuming that the concentration of POC in filtered lake water is the same as that present in ambient waters (i.e., 0.5 mg/L) is unlikely to be appropriate given that the filtering of lake water would remove most if not all of the POC present in ambient lake water. A POC concentration of 0 mg/L might be more appropriate for studies using filtered lake water. The effect of such an assumption on the BCF for BaP is discussed at the end of this section.

The third step in deriving a BCF for BaP is converting the national baseline BCFs reported for each species in each of the studies to a Florida-specific BCF. The process entails adjusting the baseline BCF which assumes all of the BaP is freely dissolved and is expressed on a 100% lipid content-basis to account for the amount of BaP that is expect to be freely dissolved in Florida surface water and for the lipid content of fish in Florida surface water. In developing its updated 2015 HHWQC USEPA used national DOC and POC concentrations and national lipid contents for fish in each of the three trophic levels. FDEP correctly recognized that the national averages were not appropriate for Florida surface waters and Florida fish and utilized Florida-specific DOC/POC and lipid concentrations. The Florida-specific DOC and POC concentrations were 12 mg/L and 0.6 mg/L, respectively, compared to the national median of 2.9 mg/L and 0.5 mg/L, respectively. The Florida-specific lipid content was 0.018, 0.015, and 0.02 in trophic levels 2, 3 and 4, respectively, compared to national average lipid contents of 0.019, 0.026, and 0.03.

USEPA's fourth step for deriving a BAF for BaP was to multiply the national BCF by a FCM. As described above, FDEP correctly recognized that application of a FCM to BaP (and to the other PAHs) is inappropriate and did not adjust the BaP BCFs beyond accounting for Florida-specific DOC and POC concentration and lipid content.

The effect of making the corrections described above (i.e., estimating fraction freely dissolved using a POC concentration of 0 mg/L, assuming the mayfly BCF reported by the study is on a freely dissolved basis) on the baseline BAF calculated by USEPA and FDEP for each species is presented in Table 2 and for the BAFs for each trophic level and the final BAF for combined trophic levels in Table 3. When all adjustments are applied, the Florida-specific BCF for BaP decreases from 596 L/kg (rounded to 600 L/kg by FDEP) to 383 L/kg. The national BAF developed by USEPA, which included the incorrect application

of FCMs, decreases from 3,875 L/kg (rounded to 3,900 L/kg by USEPA) to 2,483 L/kg. The largest contributor to the decrease in Florida-specific BCFs and the national BAFs is correcting the assumption about the concentration of POC in filtered lake water. If the three invertebrate species that are not representative of shellfish consumed by Floridians (i.e., water flea (*Daphnia magna*), amphipod (*Pontoporeia hoyi)*, and mayfly (*Hexagenia limbata*) are removed from the derivation of the Florida-specific BCF, the corrected Florida specific BCF increases from 383 L/kg (Table 2) to 484 L/kg, which is still less than the Florida-specific BCF of 600 used in the proposed HHC for BaP and the other six PAH to which the BaP BCF was applied.

Applicability of National FCMs to Florida Surface Waters and Food Webs

USEPA used a food web model (Gobas 1993) parameterized to a Great Lakes food web and fish tissue data to calculate FCMs for TLs 2, 3, and 4 (USEPA 2003). USEPA (2003) defines food chain multipliers as "a measure of the chemical's tendency to biomagnify in aquatic food webs" and provides the following equation:

$$FCM = \frac{Baseline\ BAF}{K_{ow}} \approx \frac{Baseline\ BAF}{Baseline\ BCF}$$

USEPA considered the models of both Gobas (1993) and Thomann et al. (1992) for development of FCMs, ultimately deciding to use the Gobas (1993) model for reasons described in USEPA (2003). Many of the values and assumptions used to parameterize the model for the Great Lakes are likely very different from the values and assumptions that would be used to represent surface waters and food webs in Florida.

The key input parameters are described below. Arcadis input the values and assumptions for these key parameters as described in Gobas (1993) into the spreadsheet model which is available online in an effort to reproduce the FCMs published by USEPA (USEPA 2016). Arcadis was not able to reproduce all of the FCMs and it is unclear why. Table 4 shows a comparison of the FCMs calculated using the spreadsheet model vs. those published by USEPA. In general the agreement is very close (within 5%) at log K_{ow}s less than 7, but the difference increases at higher K_{ow}s.

Sediment-Water Concentration Quotient

USEPA describes the sediment-water concentration quotient ($\prod_{socw}$) as "the ratio of the chemical concentrations in the sediments (expressed on an organic carbon basis) to those in the water column (expressed on a freely dissolved basis)". USEPA reviewed data sets from Lake Ontario, Hudson River, and Green Bay in the Lake Michigan ecosystem to determine $\prod_{socw}$. This review concluded that $\prod_{socw}$ is strongly dependent on the K_{ow} and calculated an average value of 23 for the $\prod_{socw}/K_{ow}$ ratio.

USEPA acknowledges there is very large variability in $\prod_{socw}$ across ecosystems. USEPA also presents simulations showing that constant loading results in a maximum $\prod_{socw}/K_{ow}$ of 4.9 (see Figure 4-5 of USEPA (2003)). USEPA also states that with continued loading, sediment concentration will increase until a steady state condition is reached with a $\prod_{socw}/K_{ow}$ in the 2 to 10 range. It would seem that the $\prod_{socw}/K_{ow}$ estimate of 23 is only applicable to chemicals that have high historic loading followed by a large reduction

in loading (e.g., PCBs in the Hudson River). Therefore, it is likely not applicable to most Florida waters. The $\prod_{socw}/K_{ow}$ ratio has a substantial effect on the FCMs (Table 5) because the increase in benthic tissue concentrations from sediment cause an increase in tissue concentrations that cascade up the food web.

Chemical Concentrations in Sediment and Water Column

In deriving the FCMs, 1 ng/L (concentration of chemical freely dissolved in the water column, C_w^{fd}) is used. USEPA (2003) states that the corresponding chemical concentration in the sediment is calculated by using the $\prod_{socw}/K_{ow}$ = 23 relationship, or C_s (ng/kg) = 23 (L/kg oc) * K_{ow} * (1 ng/L) * f_{oc} (kg oc/kg) * 0.001 (kg/g). The parameter is not affected by the Florida-specific values.

Organic Content of Water

To avoid using the Gobas (1993) model's method of accounting for bioavailability, USEPA (2003) set the concentration of the DOC in the model to an extremely small number, $1.0x10^{-30}$ kilograms per liter. The Gobas (1993) model takes the total concentration of the chemical in the water that is input to the model and, before doing any predictions, performs a bioavailability correction by calculating the C_w^{fd}. The C_w^{fd} is then used in all subsequent calculations by the model. By setting the concentration of the DOC to $1.0x10^{-30}$ kilograms per liter, the total concentration of the chemical input into the model becomes essentially equal to the C_w^{fd}, because the bioavailability correction employed by the method of Gobas (1993) becomes extremely small.

Rate of Metabolism in Forage and Piscivorous Fish

The FCMs developed by USEPA (USEPA 2003, 2016) assume no metabolic transformation of a compound by fish and shellfish. That is, the metabolic transformation constant (k_m) is set to zero in the model when FCMs are calculated in part because information on metabolic transformation was lacking for many compounds when the model was parameterized (i.e., in the early 1990's) and also because the model was parameterized for PCBs which are assumed to have relatively low metabolic transformation so the assumption of zero for the metabolic transformation rate constant is not unreasonable (Gobas 1993). However USEPA and FDEP are using the FCMs developed using the assumption of zero for the metabolic transformation constant to derive HHC for many compounds that differ from PCBs and are likely to be metabolized by fish or shellfish or both. Additionally a great deal more information on metabolic transformation rate constants is now available than was in the early 1990's. Arnot et al. (2008) produced a database of metabolic transformation rate constants for organic chemicals. Therefore the assumption of zero metabolism is not only incorrect, but data are available to make more appropriate assumptions, including for halogenated organics, phenyls, dioxins, and furans, hydrocarbons, amines, imides, alcohols, phenols, ethers, ketones, and esters.

To evaluate the effect of incorporating metabolism into the Gobas (1993) model used to calculate FCMs, metabolic transformation rate constants (k_m) were obtained for pentachlorophenol, heptachlor, and 1,3-dichlorobenzene (see footnotes to Table 6 for source of transformation rate constants). When the compound-specific k_ms are incorporated into the Gobas (1993) model, the FCMs for trophic levels 3 and 4 drop substantially for all three chemicals (Table 6). For pentachlorophenol and heptachlor, FDEP used FCMs greater than 1 for trophic levels 3 and 4. Because 1,3-dichlorobenzene has a log K_{ow} less than 4, FDEP defaulted to FCMs of 1 for all trophic levels. In reality, many (if not most) chemicals undergo

transformation. When transformation is accounted for and is substantial, it appears that FCMs can be less than 1.0, as demonstrated for the above three compounds.

When the FCMs calculated with metabolism are incorporated into the FDEP derivation of Florida-specific BAFs, the resulting trophic level 3 and 4 BAFs drop substantially for all three compounds (Table 6), demonstrating that incorporating metabolism, even for those chemicals that are not flagged as "highly metabolized", has a notable effect on the Florida-specific BAFs.

Additional Environmental Parameters and Conditions

USEPA (2003) used the following environmental parameters and conditions to determine FCMs:

- Mean water temperature: 8° C
- Organic carbon content of the sediment: 2.7%
- Density of lipids: 0.9 kg/L
- Density of organic carbon: 0.9 kg/L

The water temperature used by USEPA (8° C) is substantially cooler than all Florida waters. Water temperature is used in an equation that calculates the dietary uptake constant (kd) in the model. The effect of increasing temperature tends to increase the FCMs because it increases the dietary uptake (Table 5). Sediment organic carbon does not affect FCMs. Density of lipids and density of organic carbon are not water body specific assumptions and are not expected to vary between the Great Lakes and Florida surface waters.

Food Web Structure

USEPA (2003) uses the mixed food web structure from the Lake Ontario ecosystem (Flint 1986; Gobas 1993) as the representative food web for determining FCMs for the national methodology. USEPA notes that there are large differences in food webs across the country and for this reason, strongly encourages States and Tribes to make site-specific modifications to USEPA's national BAFs (USEPA 2000). Table 7 summarizes some of the key inputs used by USEPA to parameterize the food web of the Great Lakes.

Table 8 summarizes hypothetical inputs that are likely to be more representative of a food web in a Florida freshwater lake or river. Ideally, a Florida-specific food web would be calibrated to measured data. However, this hypothetical food web is presented to evaluate the potential effect of alternate food web parameters on calculated FCMs.

When the Gobas model is parameterized with assumptions and values representative of a hypothetical Florida food web rather than a Great Lakes food web, and a water temperature and sediment-water concentration quotient more representative of Florida surface waters but still assuming no metabolic transformation, the calculated FCMs increase for trophic level 3 and decrease for trophic level 4, particularly at higher K_{ow} (Table 9). Note that all of the hypothetical more Florida-specific FCMs are substantially lower than the national FCMs developed by USEPA using assumptions and values representative of surface water and food webs of the Great Lakes. While the hypothetical Florida food web and associated FCMs are presented herein purely for illustrative purposes, the results indicate that

developing a food web structure representative of Florida lakes and streams has the potential to substantially alter the calculated FCMs.

In summary, the national default assumptions used by USEPA to derive FCMs are unlikely to be representative of Florida conditions. The model is based on and calibrated for a Great Lakes food web using PCB data. As indicated above, a Florida based food web will have substantially different inputs and structure and could result in a very different outcome. In addition, assumptions of sediment contamination are based on areas that have a high historic loading followed by substantial reduction (e.g. PCBs in the Hudson River). The parameter that estimates sediment concentrations from water concentrations, $\prod_{socw}/K_{ow}$, is, therefore, higher than what would be expected in Florida waters resulting in larger FCMs than are representative of conditions in Florida. Of the parameters evaluated in the preliminary sensitivity analysis, the $\prod_{socw}/K_{ow}$ ratio has the most substantial effect of all the parameters evaluated to date (Table 5). Finally, the temperature used in the USEPA model is much cooler than might be expected in Florida waters. Inputting a higher temperature, however, tends to increase FCMs because the higher temperature results in an increase in dietary intake in the model. This increased dietary intake is not balanced by what one might expect to be an increased rate of metabolism because metabolism is assumed to be zero in USEPA's FCM model.

Summary

In summary, the preliminary evaluations presented in this white paper provide several lines of strong evidence that the application of USEPA's national BAF procedure to estimate bioaccumulation in Florida surface waters is premature and does not represent good science. Additional evaluation is necessary to identify those aspects of USEPA's national procedure that are applicable to Florida and those that need Florida-specific modification before they can be used to derive human health-based criteria for Florida surface waters. While the preliminary evaluation of some of the individual parameters of the FCM model suggest that BAFs in Florida may be lower than estimated by USEPA for the Great Lakes, the combined effect of all such modifications, and whether those will lead to higher or lower estimates of bioaccumulation, is unknown at this time.

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TABLES

Table 1. Comparison of Florida BAFs and National BAFs and Derivation Methods

CAS Number	Chemical Name	Mean Log K_{OW}	Derivation Method (for baseline BAF/BCF)	Florida BAF/BCF (L/kg-tissue)				National BAF/BCF (L/kg-tissue)			
				TL2	TL3	TL4	Alternative	TL2	TL3	TL4	Alternative
71-55-6	1,1,1-Trichloroethane	2.49	Log Kow*FCM	6	5.6	7.2	ND	6.9	9	10	ND
79-34-5	1,1,2,2-Tetrachloroethane	2.39	Log Kow*FCM	5	4.7	5.9	ND	5.7	7.4	8.4	ND
79-00-5	1,1,2-Trichloroethane	2.42	Log Kow*FCM	5.7	4.9	6.3	ND	6	7.8	8.9	ND
75-35-4	1,1-Dichloroethylene	1.73	Log Kow*FCM	2	1.8	2.1	ND	2	2.4	2.6	ND
120-82-1	1,2,4-Trichlorobenzene	4.02	Field BAFs	2,600	870	280	ND	2,800	1,500	430	ND
95-50-1	1,2-Dichlorobenzene	3.43	Log Kow*FCM	49	41	55	ND	52	71	82	ND
107-06-2	1,2-Dichloroethane	1.48	Log Kow*FCM	1.5	1.5	1.6	ND	1.6	1.8	1.9	ND
78-87-5	1,2-Dichloropropane	1.99	Log Kow*FCM	2.8	2.5	3	ND	2.9	3.5	3.9	ND
122-66-7	1,2-Diphenylhydrazine	2.94	Log Kow*FCM	17	14	18	ND	18	24	27	ND
156-60-5	1,2-Trans-Dichloroethylene	2.09	Log Kow*FCM	3	3	4	ND	3.3	4.2	4.7	ND
541-73-1	1,3-Dichlorobenzene	3.53	BCF*FCM	30	72	130	ND	31	120	190	ND
542-75-6	1,3-Dichloropropene	1.82	Log Kow*FCM	2.2	2	2.3	ND	2.3	2.7	3	ND
106-46-7	1,4-Dichlorobenzene	3.44	BCF*FCM	26	38	56	ND	28	66	84	ND
88-06-2	2,4,6-Trichlorophenol	3.69	Log Kow*FCM	88	74	98	ND	94	130	150	ND
120-83-2	2,4-Dichlorophenol	3.2	Log Kow*FCM	29	25	33	ND	31	42	48	ND
105-67-9	2,4-Dimethylphenol	2.3	Log Kow*FCM	4.6	4	5	ND	4.8	6.2	7	ND
51-28-5	2,4-Dinitrophenol	1.54	ernative BAF (BCF*F(	ND	ND	ND	3.7	ND	ND	ND	4.4
121-14-2	2,4-Dinitrotoluene	1.98	Log Kow*FCM	3	2	3	ND	2.8	3.5	3.9	ND
91-58-7	2-Chloronaphthalene	3.9	Log Kow*FCM	140	120	160	ND	150	210	240	ND
95-57-8	2-Chlorophenol	2.17	Log Kow*FCM	3.7	3.2	4	ND	3.8	4.8	5.4	ND
534-52-1	2-Methyl-4,6-Dinitrophenol	2.49	Log Kow*FCM	6.5	5.6	7.1	ND	6.8	8.9	10	ND
91-94-1	3,3'-Dichlorobenzidine	3.36	Log Kow*FCM	42	35	46	ND	44	60	69	ND
59-50-7	3-Methyl-4-Chlorophenol	3.1	Log Kow*FCM	24	20	26	ND	25	34	39	ND
50-29-3	4,4'-DDT	6.91	Field BAFs	17,000	70,000	3.9E+05	ND	35,000	240,000	1.1E+06	ND
107-02-8	Acrolein	-0.01	Log Kow*FCM	1	1	1	ND	1	1	1	ND
107-13-1	Acrylonitrile	-0.92	Log Kow*FCM	1	1	1	ND	1	1	1	ND
309-00-2	Aldrin	6.5	Log Kow*FCM	9,600	1.0E+05	2.4E+05	ND	18,000	3.1E+05	6.5E+05	ND
959-98-8	alpha-Endosulfan	3.83	Log Kow*FCM	120	100	130	ND	130	180	200	ND
71-43-2	Benzene	2.13	Log Kow*FCM	3.4	3	3.7	ND	3.6	4.5	5	ND
92-87-5	Benzidine	1.34	Log Kow*FCM	1.4	1.3	1.4	ND	1.4	1.6	1.7	ND
319-85-7	beta-BHC	3.78	Log Kow*FCM	110	91	120	ND	110	160	180	ND
33213-65-9	beta-Endosulfan	3.62	Log Kow*FCM	76	63	84	ND	80	110	130	ND
108-60-1	Bis(2-Chloro-1-Methylethyl) Eth	2.48	Log Kow*FCM	6.4	5.5	7	ND	6.7	8.8	10	ND
111-44-4	Bis(2-Chloroethyl) Ether	1.34	Log Kow*FCM	1.4	1.3	1.4	ND	1.4	1.6	1.7	ND
117-81-7	Bis(2-Ethylhexyl) Phthalate	7.5	Alternative BAF	ND	ND	ND	210	ND	ND	ND	710

Table 1. Comparison of Florida BAFs and National BAFs and Derivation Methods

CAS Number	Chemical Name	Mean Log K_{OW}	Derivation Method (for baseline BAF/BCF)	Florida BAF/BCF (L/kg-tissue)				National BAF/BCF (L/kg-tissue)			
				TL2	TL3	TL4	Alternative	TL2	TL3	TL4	Alternative
75-25-2	Bromoform	2.4	Log Kow*FCM	5.5	4.8	6	ND	5.8	7.5	8.5	ND
85-68-7	Butylbenzyl Phthalate	4.73	Alternative BAF	ND	ND	ND	11000	ND	ND	ND	19000
56-23-5	Carbon Tetrachloride	2.64	Log Kow*FCM	9	8	10	ND	9.3	12	14	ND
57-74-9	Chlordane	5.54	Log Kow*FCM	4,100	21,000	32,000	ND	5,300	44,000	60,000	ND
108-90-7	Chlorobenzene	2.84	Log Kow*FCM	13	11	15	ND	14	19	22	ND
124-48-1	Chlorodibromomethane	2.16	Log Kow*FCM	3.6	3.2	3.9	ND	3.7	4.8	5.3	ND
67-66-3	Chloroform	1.97	Log Kow*FCM	2.7	2.4	2.9	ND	2.8	3.4	3.8	ND
93-72-1	Chlorophenoxy Herbicide (2, 4, 5-TP)	3.8	Alternative BAF (BCF*FCM)	ND	ND	ND	34	ND	ND	ND	58
94-75-7	Chlorophenoxy Herbicide (2,4-D)	2.81	Alternative BAF (BCF*FCM)	ND	ND	ND	10	ND	ND	ND	13
75-27-4	Dichlorobromomethane	2.1	Log Kow*FCM	3.3	2.9	3.5	ND	3.4	4.3	4.8	ND
60-57-1	Dieldrin	6.2	Log Kow*FCM	8,200	77,000	1.7E+05	ND	14,000	210,000	4.1E+05	ND
84-66-2	Diethyl Phthalate	2.35	Alternative BAF	ND	ND	ND	580	ND	ND	ND	920
131-11-3	Dimethyl Phthalate	1.6	Alternative BAF	ND	ND	ND	2500	ND	ND	ND	4000
84-74-2	Di-n-Butyl Phthalate	4.21	Alternative BAF	ND	ND	ND	1700	ND	ND	ND	2900
1031-07-8	Endosulfan Sulfate	3.66	Log Kow*FCM	83	69	92	ND	88	120	140	ND
72-20-8	Endrin	5.47	Log Kow*FCM	3,600	17,000	25,000	ND	4,600	36,000	46,000	ND
100-41-4	Ethylbenzene	3.74	Log Kow*FCM	98	82	110	ND	100	140	160	ND
58-89-9	gamma-BHC (Lindane)	3.72	Field BAFs	1,200	1,400	1,700	ND	1,200	2,400	2,500	ND
76-44-8	Heptachlor	6.1	Log Kow*FCM	7,600	67,000	1.4E+05	ND	12,000	180,000	3.3E+05	ND
1024-57-3	Heptachlor Epoxide	5.4	Log Kow*FCM	3,200	14,000	20,000	ND	4,000	28,000	35,000	ND
87-68-3	Hexachlorobutadiene	4.78	Field BAFs	21,000	1,500	710	ND	23,000	2,800	1,100	ND
77-47-4	Hexachlorocyclopentadiene	4.52	Log Kow*FCM	570	820	850	ND	620	1500	1300	ND
67-72-1	Hexachloroethane	3.58	Field BAFs	1100	160	400	ND	1200	280	600	ND
78-59-1	Isophorone	1.67	Log Kow*FCM	1.8	1.7	1.9	ND	1.9	2.2	2.4	ND
72-43-5	Methoxychlor	4.88	Log Kow*FCM	1,200	2,600	2,800	ND	1,400	4,800	4,400	ND
74-83-9	Methyl Bromide	1.1	Log Kow*FCM	1.2	1.2	1.3	ND	1.2	1.3	1.4	ND
75-09-2	Methylene Chloride	1.3	Log Kow*FCM	1.4	1.3	1.4	ND	1.4	1.5	1.6	ND
98-95-3	Nitrobenzene	1.84	Log Kow*FCM	2.2	2	2.4	ND	2.3	2.8	3.1	ND
608-93-5	Pentachlorobenzene	5.18	Field BAFs	3,000	2,300	6,100	ND	3,500	4,500	10,000	ND
87-86-5	Pentachlorophenol	5.01	BCF*FCM	38	150	320	ND	44	290	520	ND
108-95-2	Phenol	1.46	Log Kow*FCM	1.5	1.4	1.6	ND	1.5	1.7	1.9	ND
127-18-4	Tetrachloroethylene	3.4	Log Kow*FCM	46	39	51	ND	49	66	76	ND
108-88-3	Toluene	2.72	Log Kow*FCM	10	9	11	ND	11	15	17	ND

Table 1. Comparison of Florida BAFs and National BAFs and Derivation Methods

CAS Number	Chemical Name	Mean Log K_{OW}	Derivation Method (for baseline BAF/BCF)	Florida BAF/BCF (L/kg-tissue)				National BAF/BCF (L/kg-tissue)			
				TL2	TL3	TL4	Alternative	TL2	TL3	TL4	Alternative
8001-35-2	Toxaphene	4.97	Log Kow*FCM	1,500	3,500	3,900	ND	1,700	6,600	6,300	ND
79-01-6	Trichloroethylene	2.61	Log Kow*FCM	8.3	7.1	9.1	ND	8.7	12	13	ND
75-01-4	Vinyl Chloride	1.36	Log Kow*FCM	1.4	1.3	1.5	ND	1.4	1.6	1.7	ND
83-32-9	Acenaphthene	3.98	BCF	ND	ND	ND	290	ND	ND	ND	510
120-12-7	Anthracene	4.45	BCF	ND	ND	ND	340	ND	ND	ND	610
56-55-3	Benzo (a) Anthracene	5.61	BCF	ND	ND	ND	600	ND	ND	ND	3900
50-32-8	Benzo (a) Pyrene	6.06	BCF	ND	ND	ND	600	ND	ND	ND	3900
205-99-2	Benzo (b) Fluoranthene	6.04	BCF	ND	ND	ND	600	ND	ND	ND	3900
207-08-9	Benzo (k) Fluoranthene	6.06	BCF	ND	ND	ND	600	ND	ND	ND	3900
218-01-9	Chrysene	5.16	BCF	ND	ND	ND	600	ND	ND	ND	3900
53-70-3	Dibenzo (a,h) Anthracene	6.84	BCF	ND	ND	ND	600	ND	ND	ND	3900
206-44-0	Fluoranthene	4.9	BCF	ND	ND	ND	1300	ND	ND	ND	1500
86-73-7	Fluorene	4.18	BCF	210	190	420	260	230	450	710	ND
193-39-5	Indeno (1,2,3-cd) Pyrene	6.58	BCF	ND	ND	ND	600	ND	ND	ND	3900
129-00-0	Pyrene	4.88	BCF	ND	ND	ND	370	ND	ND	ND	860
7440-41-7	Beryllium	N/A	1980 BCF	ND	ND	ND	18.9	N/A	N/A	N/A	N/A
7440-36-0	Antimony	N/A	2002 BCF	ND	ND	ND	1	N/A	N/A	N/A	N/A
57-12-5	Cyanide	0.865	2002 BCF	ND	ND	ND	1	ND	ND	ND	1
Polychlorinated Biphenyls (PCBs)		N/A	2002 BCF	ND	ND	ND	31,200	N/A	N/A	N/A	N/A
7782-49-2	Selenium	N/A	2002 BCF	ND	ND	ND	4.8	N/A	N/A	N/A	N/A

Table 2. Geometric Mean of Original and Corrected Baseline BAF Values (L/kg-lipid)

TL	Species	N	EPA Baseline (Original)	EPA Baseline (Corrected)	FL Baseline (Original)	FL Baseline (Corrected)
2	Amphipod (Pontoporeia hoyi)	1	2,470,769	**1,342,467**	2,470,769	**1,342,467**
2	Mayfly (Hexagenia limbata)	1	360,081	**195,633**	360,081	**195,633**
2	Shrimp (Mysis relicta)	1	808,223	**439,118**	808,223	**439,118**
2	Water flea (Daphnia magna)	1	294,452	**202,600**	294,452	**202,600**
2	Zebra mussel (Dreissena polymorpha)	19	2,252,602	**1,549,961**	2,252,602	**1,549,961**
2	Bluegill sunfish (Lepomis macrochirus)	4	120,798	**83,079**	11,824	**8,132**

Table 3. Geometric Mean of Original and Corrected Final BAF Values (L/kg-tissue)

TL	EPA (Final)	**EPA Final (Corrected)**	FL (Final)	**FL Final (Corrected)**
2	8,848	5,284	5,562	3,321
3	1,697	1,167	64	44
2/3	3,875	2,483	596	383

Table 4. Comparsison of Gobas Speadsheet Results and USEPA Published Values

Gobas Model Parameter	Log Kow	4	5	6	7	8	9
	Water Temperature	8^{o} C (National Default Temperature)					
	SOWC/Kow	23					
Model Calculated Food Chain Multipliers	TL2	1	1	1	1	1	1
	TL3	1.23	3.01	9.87	13.8	9.19	1.99
	TL4	1.07	2.49	14.7	25.6	10.6	0.44
Food Chain Multipliers, EPA (2003) Table 4-6	TL2	1	1	1	1	1	1
	TL3	1.23	3	9.79	13.2	7.6	1.38
	TL4	1.07	2.51	14.9	24.3	7.23	0.21

Table 5. Sensitivity of Various Gobas Model Parameters With Respect to Calculated Food Chain Multipliers

Gobas Model Parameter	Log Kow	5							
	Water temperature	8° C (National Default Temperature)				16° C (Alternative Florida)			
	SOWC/Kow	23 (Default)	10	5	2	23 (Default)	10	5	2
Model Calculated Food Chain Multipliers	TL2	1	1	1	1	1	1	1	1
	TL3	3.01	1.86	1.42	1.15	4.08	2.34	1.66	1.26
	TL4	2.49	1.82	1.57	1.41	3.99	2.60	2.06	1.74
Gobas Model Parameter	Log Kow	6							
	Water temperature	8° C (National Default Temperature)				16° C (Alternative Florida)			
	SOWC/Kow	23 (Default)	10	5	2	23 (Default)	10	5	2
Model Calculated Food Chain Multipliers	TL2	1	1	1	1	1	1	1	1
	TL3	9.87	4.81	2.85	1.66	12.5	5.97	3.47	1.94
	TL4	14.7	7.45	4.67	3.00	22.8	11.2	6.80	4.14
Gobas Model Parameter	Log Kow	7							
	Water temperature	8° C (National Default Temperature)				16° C (Alternative Florida)			
	SOWC/Kow	23 (Default)	10	5	2	23 (Default)	10	5	2
Model Calculated Food Chain Multipliers	TL2	1	1	1	1	1	1	1	1
	TL3	13.8	6.4	3.6	1.9	16.1	7.5	4.2	2.2
	TL4	25.6	12.2	7.1	4.0	36.0	17.1	9.8	5.5

Table 6. Comparison of FCMs and BAFs Calculated With and Without Metabolism

Parameter	Trophic Level	Without Metabolism	With Metabolism
Pentachlorophenol	**log k_{ow} = 5.01**	**k_m = 1.66 day^{-1} [a]**	
FCM	**TL2**	1.0	1.0
	TL3	3.0	0.13
	TL4	2.6	0.0037
BAF/BCF	**TL2**	38	38
	TL3	150	7.4
	TL4	320	1.3
Heptachlor	**log k_{ow} = 6.10**	**k_m = 0.025 day^{-1} [b]**	
FCM	**TL2**	1.0	1.0
	TL3	11	4.1
	TL4	17	0.91
BAF/BCF	**TL2**	7600	7600
	TL3	67000	26000
	TL4	140000	7700
1,3-Dichlorobenzene	**log k_{ow} = 3.53**	**k_m = 0.578 day^{-1} [b]**	
FCM	**TL2**	1.0	1.0
	TL3	1.0	0.82
	TL4	1.0	0.22
BAF/BCF	**TL2**	30	30
	TL3	72	59
	TL4	130	29

a. Hazardous Substances Data Bank
(https://toxnet.nlm.nih.gov/cgi-bin/sis/search2/r?dbs+hsdb:@term+@DOCNO+894)

b. Arnot et al. (2008)

Table 7. Lake Ontario Based Food Web Model Used to Derive National Food Chain Multipliers Adopted by FDEP

Species	Trophic Level	Lipid Content	Weight	Diet
Phytoplankton	1	0.5%	--	--
Zooplankton (mysids [*Mysis relicta])*	2	5%	100 mg	--
Benthic Invertebrates (*Diporeia)*	2	3%	12 mg	--
Sculpin (*Cottus cognatus)*	3	8%	5.4 g	18% zooplankton, 82% *Diporeia*
Alewife (*Alosa pseudoharengus)*	3	7%	32 g	60% zooplankton, 40% *Diporeia*
Smelt (*Osmerus mordax*)	3-4	4%	16 g	54% zooplankton, 21% *Diporeia* , 25% sculpin
Salmonids (*Salvelinus namaycush, Oncorhynchus mykiss, Oncorhynchus velinus namaycush*	4	11%	2,410 g	10% sculpin, 50% alewife, 40% smelt

Table 8. Hypothetical Florida-Based Food Web Model Parameters

Species	Trophic Level	Lipid Content	Weight	Diet
Phytoplankton	1	0.5%	--	--
Zooplankton (mysids [*Mysis relicta])*	2	5%	100 mg	--
Crayfish	2	1%	6 g	--
Panfish (sunfish)	3	3%	200 g	20% zooplankton, 80% crayfish
Largemouth bass	4	4%	2,000 g	20% crayfish, 80% panfish
Freshwater catfish	4	8%	5,000 g	20% crayfish, 80% panfish

Table 9. Comparison of FCMs Calculated With Great Lakes and Hypothetical Florida Food Web Parameters

Gobas Model Parameter	Log Kow	4	5	6	7
	Water Temperature	16° C (Alternative Florida)			
	SOWC/Kow	5			
Great Lakes Food Web	TL2	1	1	1	1
	TL3	1.1	1.7	3.5	4.2
	TL4	1.1	2.1	6.8	9.8
Hypothetical Florida Food Web	TL2	1	1	1	1
	TL3	1.1	1.7	3.8	4.9
	TL4	1.1	1.7	5.2	7.1

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ATTACHMENT F

Review of PAH Bioaccumulation and Bioconcentration Factors used by USEPA in Derivation of 2015 Human Health Water Quality Criteria

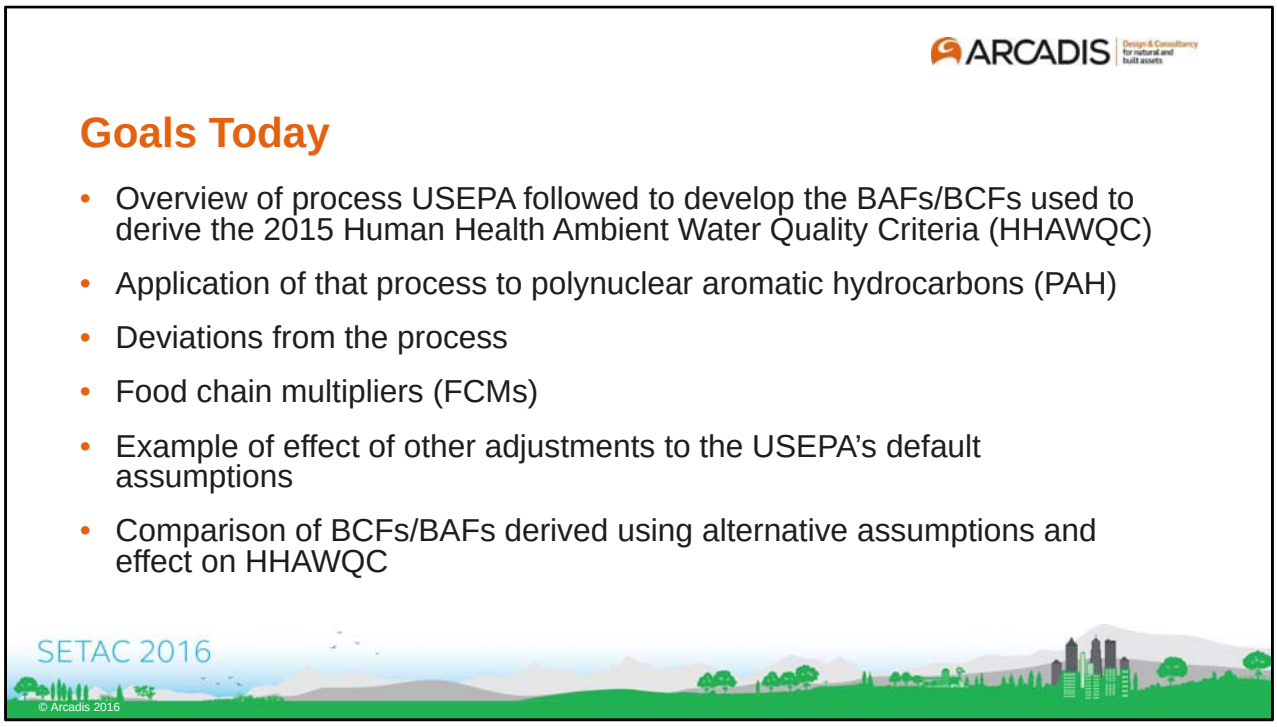
This attachment presents annotated slides from a platform presentation on November 10, 2017 at the 37th Annual Meeting of the Society of Environmental Toxicology and Chemistry held in Orlando, Florida. The slides are the same as those presented at the conference. The text associated with each slide has been added since the platform presentation to provide context and explanation.

REVIEW OF PAH BIOACCUMULATION AND BIOCONCENTRATION FACTORS USED BY USEPA IN DERIVATION OF 2015 HUMAN HEALTH WATER QUALITY CRITERIA

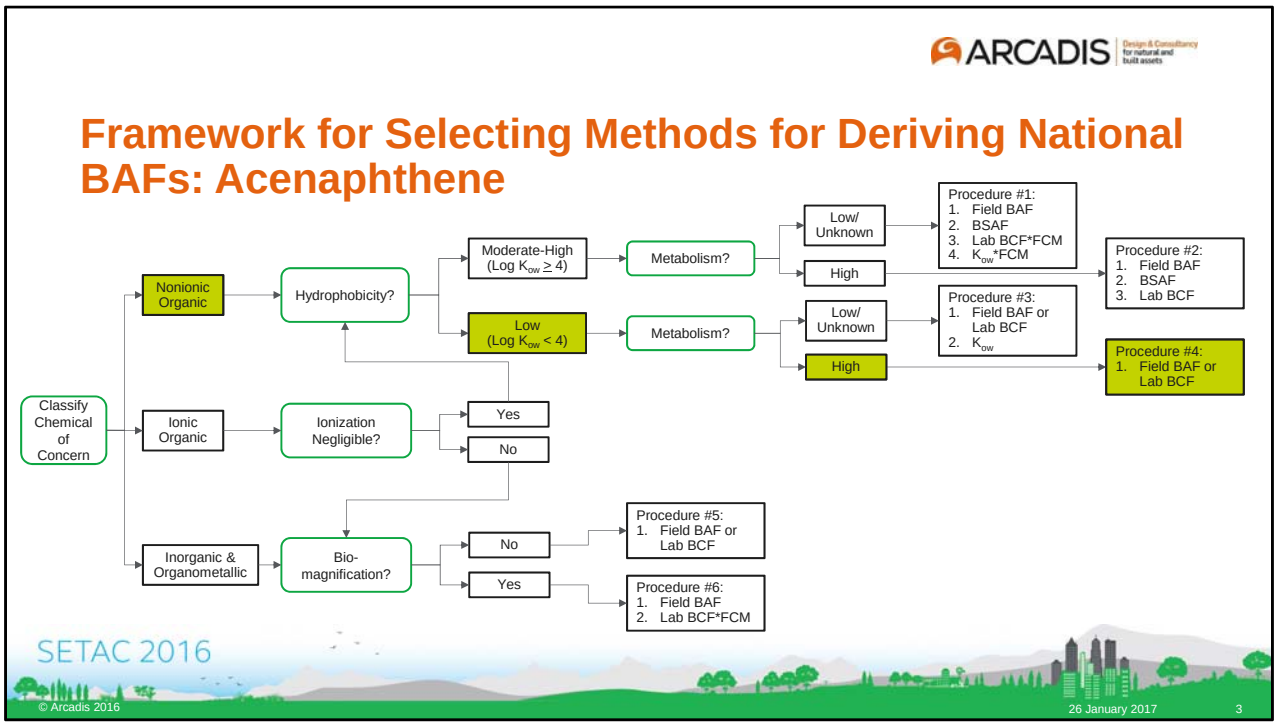
Paul Anderson, Jacqueline Iannuzzi, Michele Buonanduci

November 10, 2016

This presentation reviews the bioaccumulation/bioconcentration methodology employed by USEPA to derive the 2015 human health ambient water quality criteria (HHAWQC) and released by USEPA in January 2016. The presentation uses polynuclear aromatic hydrocarbons (PAH) as example compounds. However, many of the topics described in the presentation are applicable to other compounds for which USEPA derived HHAWQC in 2015.



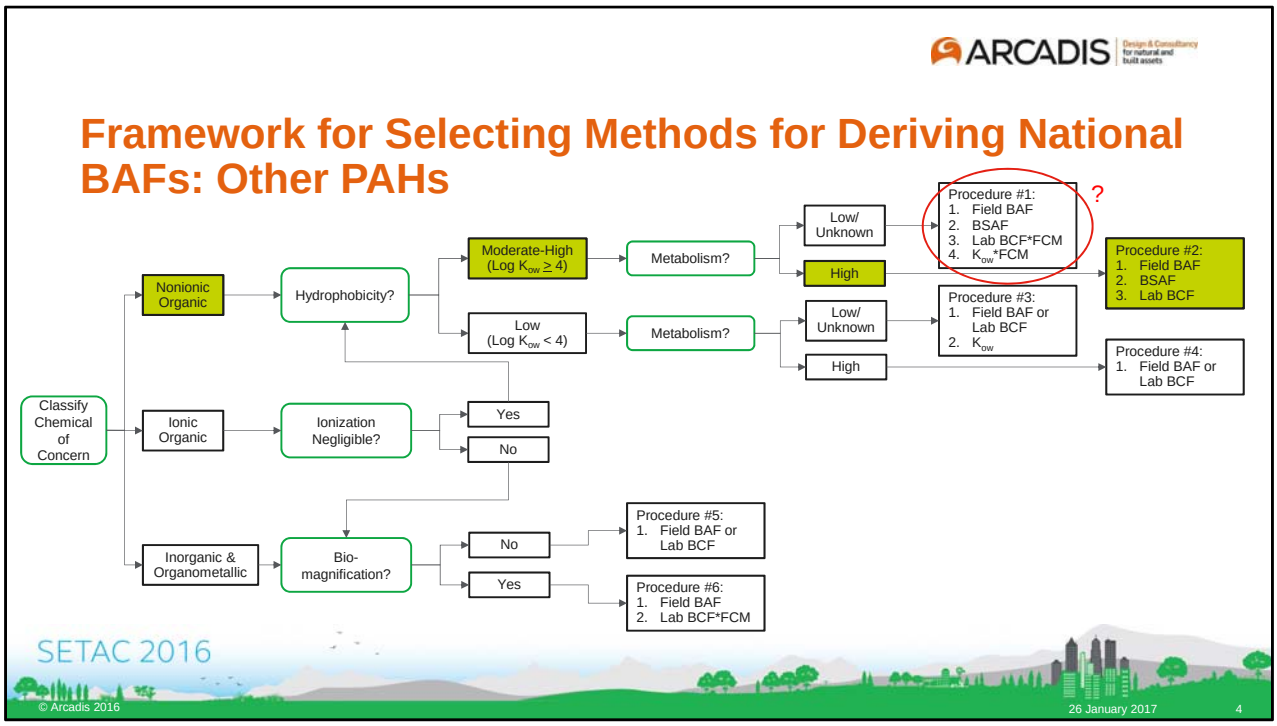
The presentation will review the overall process followed by USEPA to develop bioaccumulation factors (BAFs) and bioconcentration factors (BCFs) used to derive the 2015 HHAWQC. PAH are used as the example class of compounds to which BAF/BCF methodology was applied. The application to PAH will document ways in which USEPA deviated from the process it describes in the January 2016 methodology. The presentation also touches on the purpose, application and applicability of food chain multipliers (FCMs) to PAH. It also presents a summary of some of the other assumptions that might be appropriate to adjust before using the 2015 BAFs/BCFs when setting State-specific HHAWQC. The presentation concludes by showing how the BAFs/BCFs used by USEPA in the 2015 PAH HHAWQC can change when some of these changes are incorporated into the derivation process.



USEPA's framework for selecting a method to derive national BAFs is presented in this slide. The framework contains three decision points.

- The first is identifying whether the chemical is organic and, if it is organic, whether it is ionized in ambient surface waters.
- Second, if the compound is an organic and it is not ionized in ambient surface waters, whether the chemical has a low or moderate-high K_{ow}, where the threshold between the two categorizations of low versus moderate-high is a log K_{ow} of 4.
- Third, for non-ionized organic chemicals the degree of metabolism affects the procedure that is selected to estimate the BAF.

The boxes highlighted in green present the outcome of the above decision points for acenaphthene. USEPA classifies acenaphthene as a nonionic organic chemical with low K_{ow} and high metablolism. That results in the national BAF being based on Procedure #4, in which the national BAF is based either on a field-measured BAF or a laboratory-measured BCF. USEPA used Procedure #4 to derive the National BAF for acenaphthene.



USEPA's framework for selecting a method to derive national BAFs is presented in this slide with boxes highlighted for seven PAH for which benzo(a)pyrene is assumed to be a surrogate. USEPA classifies these seven PAH as nonionic organic chemicals with moderate-high K_{ow} and high metabolism. Based on the framework, that should result in the national BAF being based on Procedure #2, in which the national BAF is based either on a field-measured BAF, a BSAF, or a laboratory-measured BCF. However, despite the above classifications, when developing national BAFs for these seven PAH, USEPA elected to use Procedure #1 (circled in red on the slide). In that procedure, the national BAF is based either on a field-measured BAF, a BSAF, a laboratory-measured BCF multiplied by a FCM, or the K_{ow} multiplied by the FCM. USEPA does not provide an explanation for the deviation from the framework, though as described in subsequent slides, the effect on the final national BAF can be quite large.

Food Chain Multipliers

- BCFs theoretically account for uptake from only water
- FCMs used to account for uptake from other exposure pathways (e.g. diet, sediment)
- USEPA 2016 FCMs based on modeling of Great Lakes foodweb
- Great Lakes are unique and may not be representative of many other US waters
- USEPA 2016 FCMs do not include metabolic transformation, hence why USEPA's process indicates FCMs should not be used for highly metabolized compounds

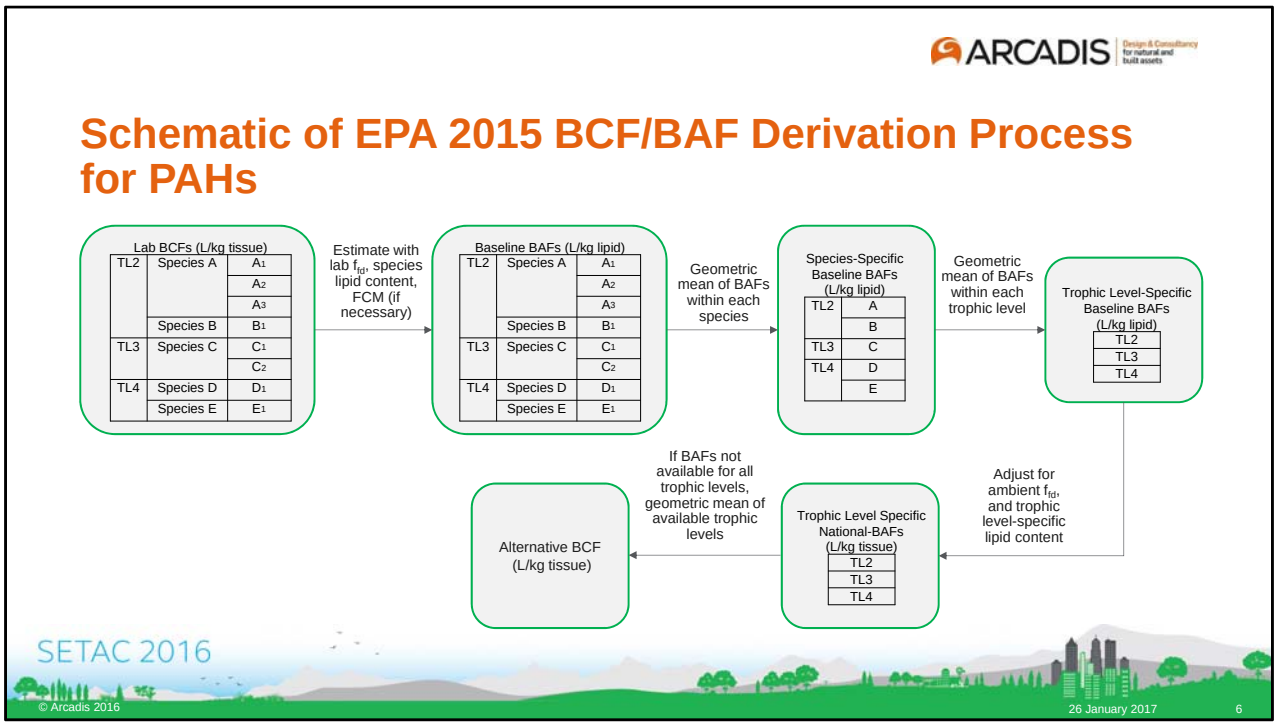
Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4	Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4	Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
4.0	1	1.23	1.07	5.7	1	7.40	9.54	7.4	1	12.0	19.5
4.1	1	1.29	1.09	5.8	1	8.21	11.2	7.5	1	11.5	17.6
4.2	1	1.36	1.13	5.9	1	9.01	13.0	7.6	1	10.8	15.5
4.3	1	1.45	1.17	6.0	1	9.79	14.9	7.7	1	10.1	13.3
4.4	1	1.56	1.23	6.1	1	10.5	16.7	7.8	1	9.31	11.2
4.5	1	1.70	1.32	6.2	1	11.2	18.5	7.9	1	8.46	9.11
4.6	1	1.87	1.44	6.3	1	11.7	20.1	8.0	1	7.60	7.23
4.7	1	2.08	1.60	6.4	1	12.2	21.6	8.1	1	6.73	5.58
4.8	1	2.33	1.82	6.5	1	12.6	22.8	8.2	1	5.88	4.19
4.9	1	2.64	2.12	6.6	1	12.9	23.8	8.3	1	5.07	3.07
5.0	1	3.00	2.51	6.7	1	13.2	24.4	8.4	1	4.33	2.20
5.1	1	3.43	3.02	6.8	1	13.3	24.7	8.5	1	3.65	1.54
5.2	1	3.93	3.68	6.9	1	13.3	24.7	8.6	1	3.05	1.06
5.3	1	4.50	4.49	7.0	1	13.2	24.3	8.7	1	2.52	0.721
5.4	1	5.14	5.48	7.1	1	13.1	23.6	8.8	1	2.08	0.483
5.5	1	5.85	6.65	7.2	1	12.8	22.5	8.9	1	1.70	0.320
5.6	1	6.60	8.01	7.3	1	12.5	21.2	9.0	1	1.38	0.210

SETAC 2016

This slide provides some background on FCMs. The embedded table presents the FCMs used by USEPA to derive national BAFs. The concept of the FCM arose from the realization that, theoretically, BCFs only account for uptake of a chemical by aquatic biota directly from water. For many chemicals, other exposure pathways are present and can make a substantial contribution to uptake from the aquatic environment, such as diet and sediment. FCMs were developed to account for these other uptake pathways. The FCMs were based on a model of the accumulation of polychlorinated biphenyls (PCBs) in the Great Lakes food web.

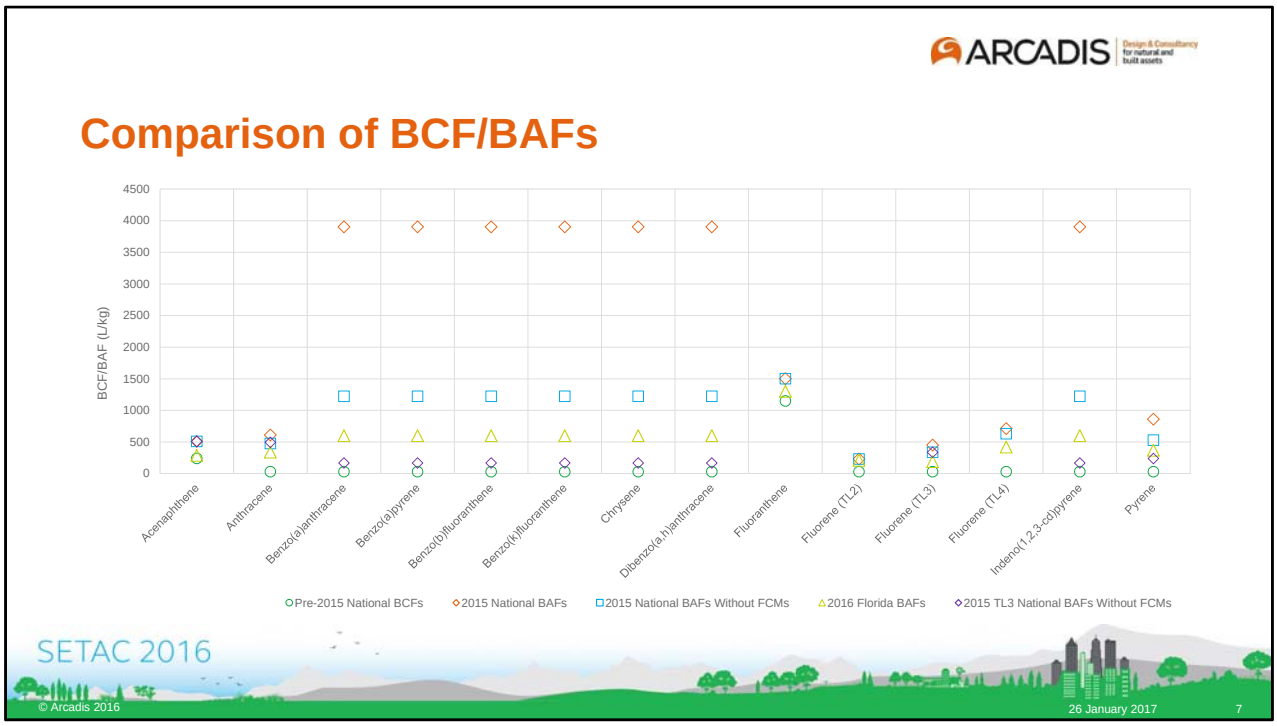
As shown in the table, FCMs are close to 1 for chemicals with a log K_{ow} of about 4 (i.e., pathways other than direct uptake from water contribute little to overall exposure meaning that total accumulation is only slightly greater than that predicted by a BCF). FCMs increase with increasing log K_{ow}, to a maximum about 13 for trophic level 3 and 25 for trophic level 4 near a log K_{ow} of 7 (i.e., pathways other than direct uptake from water contribute about 13 and 25 times more to overall exposure for these two trophic levels than just direct uptake from water). At log K_{ow}s of greater than 7, FCMs decrease with increasing log K_{ow} and approach or are less than 1 at a log K_{ow} of 9. The effect of K_{ow} on predicted FCM is why USEPA's framework contains a K_{ow}-based decision point; at log K_{ow}s of less than 4, exposure from exposure pathways other than direct uptake from water do not need to be account for.

In addition to K_{ow}, metabolism also plays a significant role in bioaccumulation of chemicals in aquatic biota. Specifically, accumulation of metabolized chemicals can be substantially lower than accumulation of non-metabolized chemicals. The model used by USEPA to develop the FCMs is based on PCBs and assumes no metabolism of PCBs. Thus, the FCMs are applicable to only compounds that have no or little metabolism and is the reason the framework includes a metabolism-based decision point. FCMs for metabolized compounds, such as PAHs, would be expected to be lower, perhaps substantially lower, than the FCMs shown in the above table.



A schematic of USEPA's application of the framework to derive national BAFs for PAHs is presented in this slide.

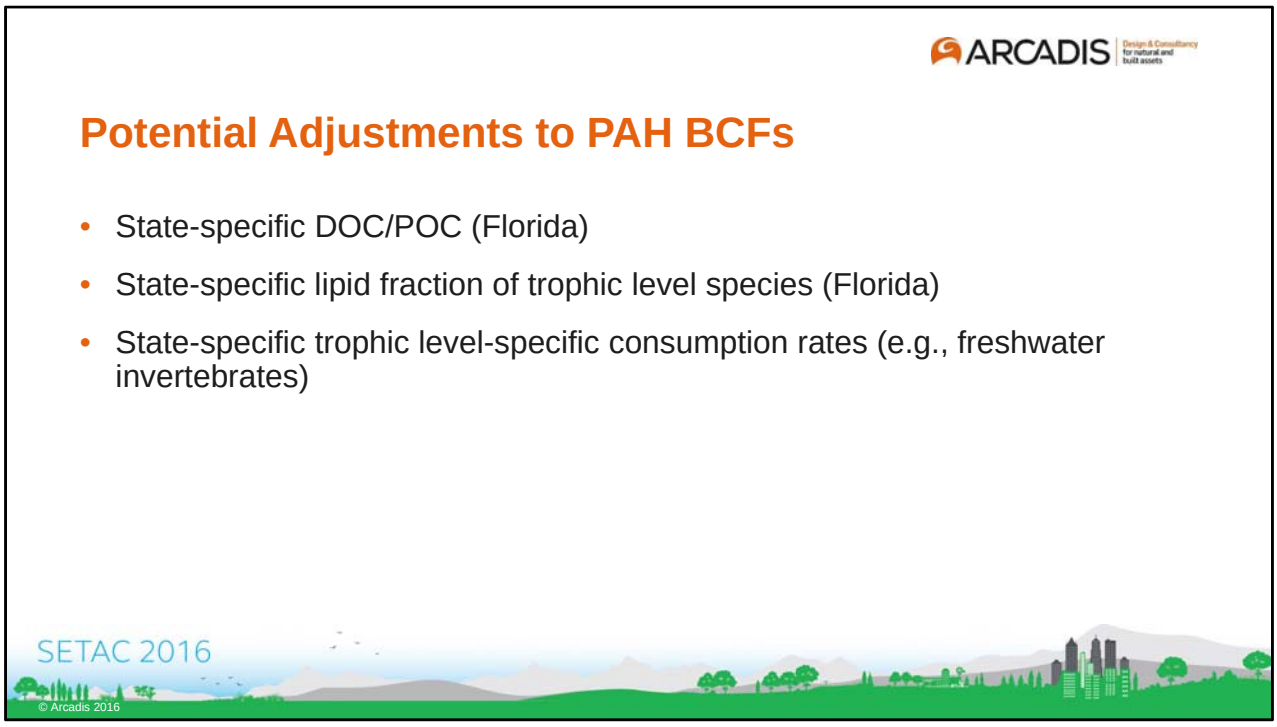
- The process starts with a listing of all laboratory BCFs for a specific PAH included in USEPA's database. Each measured BCF is categorized by species and trophic level.
- Each laboratory measured BCF is then converted to a Baseline BAF (expressed on a freely dissolved, 100% lipid basis). If called for by the framework, a laboratory measured BCF is multiplied by a FCM.
- For each species that has more than one Baseline BAF, the species-specific Baseline BAF is estimated by taking the geometric mean of all the Baseline BAFs measured for that species.
- For each trophic level that has more than one species-specific Baseline BAF, a Trophic Level-specific Baseline BAF is estimated by taking the geometric mean of all the species-specific BAFs measured for that trophic level.
- Trophic level-specific Baseline BAFs are converted to Trophic Level-specific National BAFs by adjusting the Baseline BAFs to account for the trophic level-specific lipid content of fish in national surface waters and fraction freely dissolved of each chemical in national surface waters. When National BAFs are available for all trophic levels, they are used to develop National HHAWQC. As discussed in subsequent slides, USEPA's framework identifies fraction freely dissolved and trophic level-specific lipid adjustments to make BAFs more water body-specific.
- If National BAFs are absent for one or more trophic levels, the geometric mean of the available Trophic Level-specific National BAFs is used to derive National HHAWQC.



This graph shown on the slide plots several different BCFs/BAFs (as described below) for 12 PAH. The value of the BCF/BAF is shown on the y-axis and the name of each PAH is shown on the x-axis. Note that fluorene is shown three times on the x-axis corresponding the availability of BAFs for all three trophic levels.

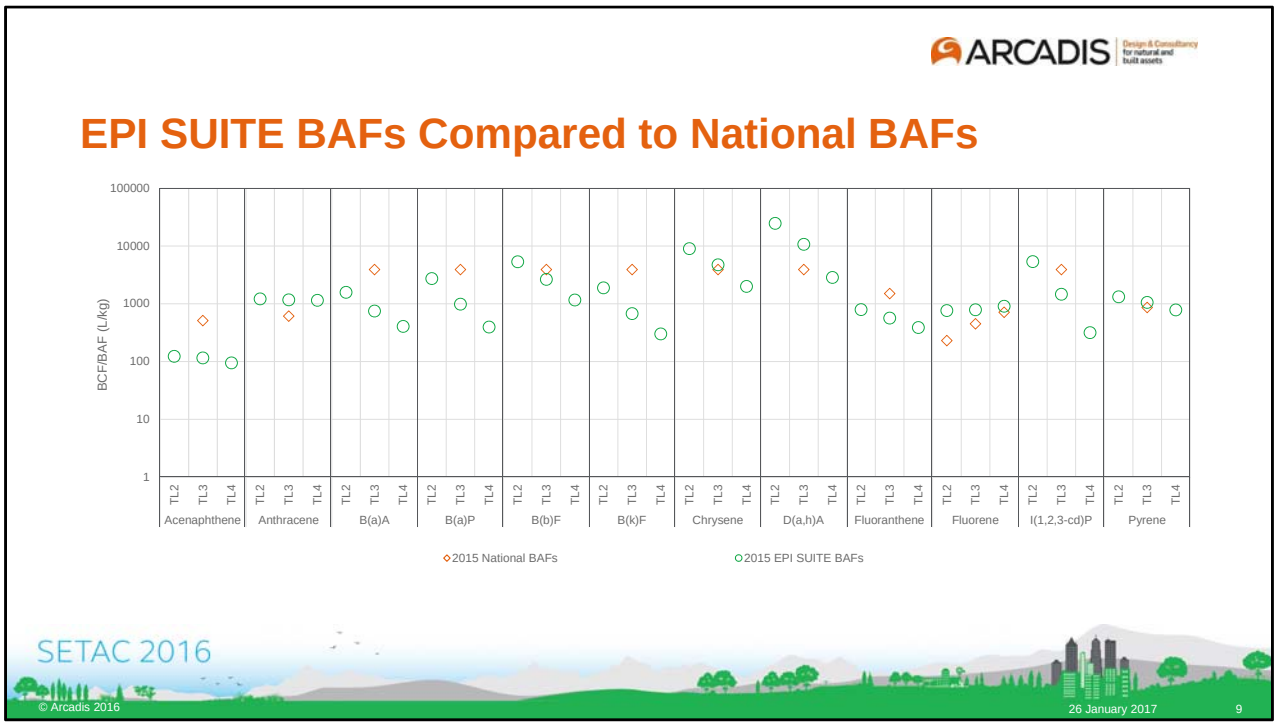
- The green circles present the BCF used to derive National HHAWQC prior to issuance of the new 2015 HHAWQC. For all PAH, these are the lowest BCF/BAFs shown on the figure. With the exception of acenaphthene and fluoranthene, the BCFs were uniform and low (30 L/kg).
- The orange diamonds present the BAF used to derive the 2015 National HHAWQC. For all PAH, these are the highest BAFs shown on the figure. For seven PAH, these are identical because the bioaccumulation of benzo(a)pyrene is used as a surrogate to represent the bioaccumulation of the other six PAH.
- The blue squares present the BAFs that would result if the FCM was not applied to the derivation of the National BAF. As described above, USEPA classifies all 12 PAH as having high metabolism. Based on the BAF framework presented in USEPA's BAF guidance (USEPA 2016) a FCM should not have been applied in the derivation of the National BAFs for PAH. The National BAF for the seven PAH represented by benzo(a)pyrene would be about three times lower than the National BAF used by USEPA in the 2015 HHAWQC, and the resulting HHAWQC would have been about three times higher. The effect of the FCM is less for the other three PAH to which it was applied (i.e., anthracene, fluorene, pyrene).
- Green diamonds present the BAF used by the Florida Department of Environmental Protection (FDEP) to derive their proposed State-specific HHAWQC. In addition to not applying a FCM when deriving BAFs for PAH, FDEP also used Florida-specific information on the lipid content of fish and dissolved and particulate organic carbon (DOC and POC) in Florida waters to derive a Florida-specific BAF from USEPA's baseline BAF for each PAH. The Florida-specific BAFs are lower for all PAH than National BAFs derived without using a FCM. The largest difference occurs for the seven PAH represented by benzo(a)pyrene. The Florida-specific BAFs are about 6.5 times lower than the National BAF used by USEPA in the 2015 HHAWQC.
- The purple diamonds represent National BAFs for the Trophic Level 3 derived without using a FCM. For most PAH, these BAFs end up being the lowest of all the BAFs based on the information used by USEPA to derive BAFs for the 2015 HHAWQC. The purpose of these BAFs is to demonstrate the effect on the

National BAF of excluding the accumulation of PAH measured for Trophic Level 2 aquatic biota which consist of invertebrates (e.g. shellfish). While consumption of invertebrates in ambient waters is likely from estuaries of coastal states, consumption of invertebrates from local freshwaters is infrequent in inland states. It turns out that because most invertebrates do not metabolize PAH, they bioaccumulate PAH at substantially higher rates than finfish. Consequently, when Trophic Level 2 BAFs (i.e., most invertebrates) are excluded from the derivation of a National BAF, the National BAF decreases substantially. A combined Trophic Level 3 and 4 National BAF is not shown on the figure because USEPA's database does not contain data on BCFs for PAH measured in Trophic Level 4 species.



As suggested by the previous slide, several adjustments to the National BAFs could make them more applicable to a State's surface waters. The list shown on this slide is not comprehensive. It focuses on adjustments that could be made based on State-specific information.

- The concentration of DOC and POC in surface water can be used to develop a State-specific estimate of the fraction of freely dissolved chemical in surface waters. Many States are likely to have such data (see FDEP 2016). Such data can be applied to estimate a State-specific fraction freely dissolved for all organic chemicals, not just PAH.
- Some States may also have data on the lipid content of species in different trophic levels. The State-specific lipid data can be used to develop State-specific lipid fractions for each trophic level (see FDEP 2016).
- Although not a specific adjustment called out by USEPA's BAF framework, the National BAFs assume consumption of a specific amount of fish from each of three trophic levels. As noted above, trophic level 2 consists of invertebrates but consumption of aquatic invertebrates from freshwater is a relatively rare occurrence, certainly much less frequent than the consumption of shellfish such as shrimp, crabs, clams and lobster that comprise the majority of trophic level 2 species included in the National BAF trophic level 2 fish consumption rate. States should consider deriving State-specific HHAWQC based on trophic level-specific fish consumption rates that reflect the species present in and consumed from State waters.



The graph shown on the slide plots two sets of BAFs for the 12 PAH for which USEPA proposed HHAWQC in 2015. The value of the BAF is shown on the y-axis and the name of each PAH on the x-axis. The green circles present the trophic level-specific BAF derived using EpiSuite for each of the PAH. The orange diamonds present the National BAF used by USEPA to derive the 2015 HHAWQC. EpiSuite is a model used by USEPA to estimate bioaccumulation for different compounds across the three trophic levels. The EpiSuite model accounts for metabolism and some other parameters that may make it a better predictor of BAFs than the FCM model USEPA used in the framework to derive the National BAFs used to develop the 2015 HHAWQC. The EpiSuite BAFs are presented in the supporting documentation for each individual PAH.

Review of the 2015 National BAFs and the EpiSuite BAFs for PAH reveals some general trends and observations.

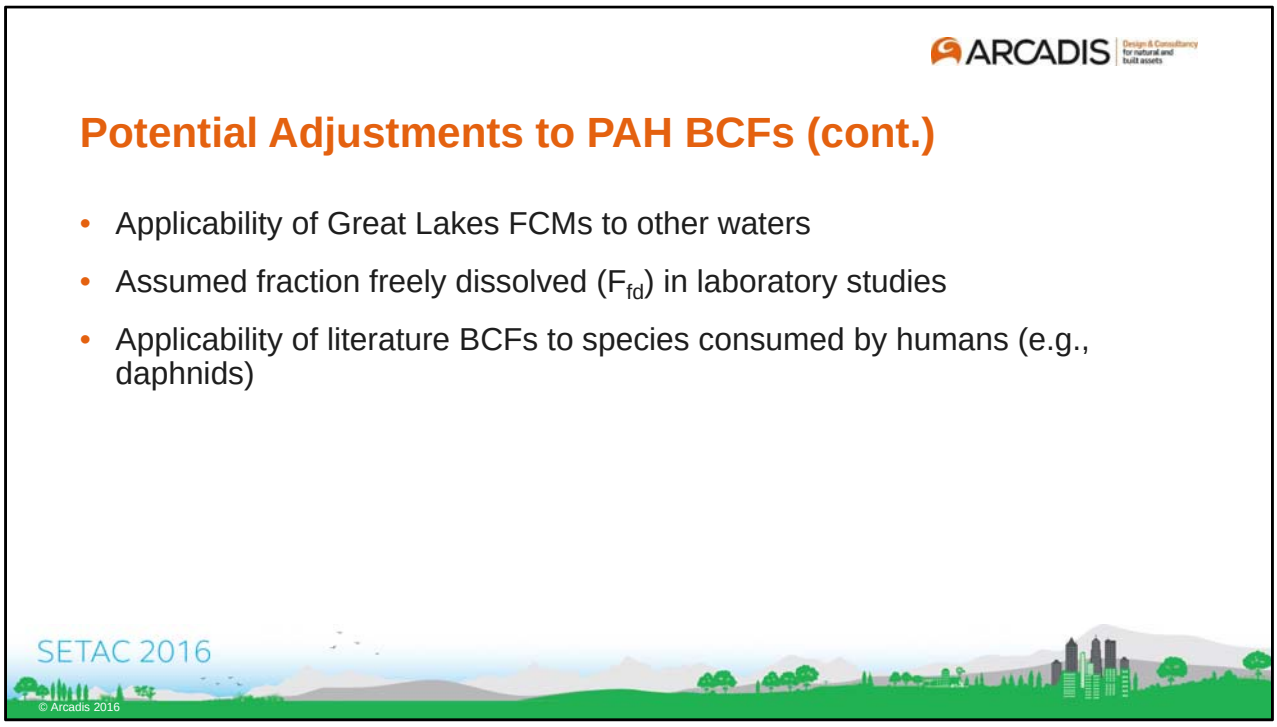
- For most PAH, fluorene being the exception, EpiSuite BAFs decrease with increasing trophic level. This is consistent with the expectation that PAH are metabolized and points to why FCMs, which predict increasing concentrations of PAH (and all other chemicals) with increasing trophic level, are not appropriate to use for chemicals such as PAH that are metabolized.
- For five PAH, all three trophic level-specific BAFs are lower than the 2015 National BAF. For most PAH the trophic level 3 and 4 EpiSuite BAFs are lower than the 2015 National BAF. Only fluorene has 2015 National BAFs lower than the EpiSuite BAFs for all trophic levels. The comparison suggests that the 2015 National BAFs overestimate bioaccumulation of PAH and may lead to lower HHAWQC than would be derived if USEPA's 2016 BAF methodology had been followed by USEPA when developing the 2015 HHAWQC.

Individual PAH supporting documentation:

- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Acenaphthene, 83-32-9. EPA 820-R-15-002. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0234
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Anthracene, 120-12-7. EPA 820-R-

15-008. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0236

- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Benzo(a)anthracene, 56-55-3. EPA 820-R-15-011. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0176
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Benzo(a)pyrene, 50-32-8. EPA 820-R-15-012. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0177
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Benzo(b)fluoranthene, 205-99-2. EPA 820-R-15-013. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0178
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Benzo(k)fluoranthene, 207-08-9. EPA 820-R-15-014. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0179
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Chrysene, 218-01-9. EPA 820-R-15-030. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0184
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Dibenzo(a,h)anthracene, 53-70-3. EPA 820-R-15-032. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0185
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Fluoranthene, 206-44-0. EPA 820-R-15-043. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0220
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Fluorene, 86-73-7. EPA 820-R-15-044. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0221
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Indeno(1,2,3-cd)pyrene, 193-39-5. EPA 820-R-15-053. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0187
- USEPA. 2015. Update of Human Health Ambient Water Quality Criteria: Pyrene, 129-00-0. EPA 820-R-15-062. Office of Water, Office of Science and Technology. June. https://www.regulations.gov/document?D=EPA-HQ-OW-2014-0135-0248



States may want to consider other adjustments to the framework and USEPA's application of the framework that do not require State-specific data but, rather, involve refinements to the data used by USEPA or the framework itself.

- As described in other attachments, the most important consideration may be the applicability of the food chain model USEPA used to derive FCMs. That model was based on PCBs in the Great Lakes. PCBs are not representative of all compounds to which FCMs may be applied and the Great Lakes are not representative of all waters of the United States.
- In the absence of data on the fraction of freely dissolved chemicals in laboratory BCF experiments, USEPA assumed the concentration of DOC and POC in test aquaria was the same as the average concentration in national ambient waters. If water in the test aquaria was filtered or treated in some way prior to use, it is possible, if not likely, that DOC and especially POC concentrations are lower than found in natural waters. If that were to be the case, then the fraction freely dissolved would be greater than USEPA estimated and the Baseline BAFs lower than USEPA reports.
- Several of the BCFs that USEPA includes in its database are measured in invertebrate species (such as daphnids) that are not consumed by humans. Before using such data, States may want to confirm BCFs reported for such species are representative BCFs in species regularly consumed by people.
- The completeness of USEPA's BCF/BAF database and the frequency at which it is updated is unclear. States may wish to review and update the data for key compounds of interest when deriving or updating State-specific HHAWQC.

Although not an adjustment used to derive National BAFs from the information presented in USEPA's database or a refinement of that process, some States may have State-specific information on bioaccumulation of chemicals in their waters. As indicated in the framework, a field BAF is the preferred measure of bioaccumulation when deriving HHAWQC. Such BAFs could be used in place of the BAFs estimated using the BAF derivation process presented in USEPA's 2016 guidance.

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Effect on HHAWQC

Compound	Pre-2015 National HHAWQC (ug/L)	2015 National HHAWQC (ug/L)		
		Using 2015 National BAFs	Using 2015 National BAFs Without FCMs	Using 2015 National TL3 BAFs Without FCMs
Acenaphthene	670	70	70	70
Anthracene	8300	300	370	360
Benzo(a)anthracene	0.0038	0.0012	0.0037	0.018
Benzo(a)pyrene	0.0038	0.00012	0.00037	0.0018
Benzo(b)fluoranthene	0.0038	0.0012	0.0037	0.018
Benzo(k)fluoranthene	0.0038	0.012	0.037	0.18
Chrysene	0.0038	0.12	0.37	1.8
Dibenzo(a,h)anthracene	0.0038	0.00012	0.00037	0.0018
Fluoranthene	130	20	20	NA
Fluorene	1100	50	60	67
Indeno(1,2,3-cd)pyrene	0.0038	0.0012	0.0037	0.018
Pyrene	830	20	30	63

SETAC 2016

This table presents a comparison pf the pre-2015 HHAWQC to the 2015 HHAWQC for 12 PAH. The first column presents the name of each PAH included in the comparison. The second column presents the pre-2015 HHAWQC for 12 PAH. The third column presents the 2015 HHAWQC as derived by USEPA. The fourth column presents the 2015 HHAWQC without the FCM. The fifth column presents the 2015 HHAWQC without the FCM and based on only the Trophic Level 3 BAF. With the exception of benzo(k)fluoranthene and chrysene, the 2015 HHAWQC are lower than the pre-2015 HHAWQC. For about half of the PAH, the decrease is about 10-fold (or more). HHAWQC based on BAFs that do not include the FCM or that are based on only Trophic Level 3 BAFs are greater than the 2015 HHAWQC for most PAH, but are still lower than the pre-2015 HHAWQC for about seven of the 12 PAH.

Summary

- USEPA did not follow its own guidance when deriving BAFs/alternative BCFs for PAH and the 2015 national HHAWQC
- USEPA used FCMs to adjust BCFs of 11 of 12 PAH even though guidance indicates FCMs should not be used for highly metabolized compounds
- 2015 national HHAWQC for most PAH increase when FCMs are removed from derivation – about 3.5 times higher for 7 of 12 PAH
- Other refinements also likely warranted (e.g., state-specific DOC/POC concentrations and trophic level lipid content)
- Combined, these could lead to substantially lower HHAWQC

In summary, USEPA did not follow the framework presented in its own guidance when deriving BAFs for 11 of the 12 PAH for which updated HHAWQC were recommended in 2015 because it used FCMs to adjust BCFs for those PAH even though guidance indicates FCMs should not be used for highly metabolized compounds. The 2015 national HHAWQC for most PAH increase when FCMs are removed from the HHAWQC derivation and increase by slightly more than 3-fold for the seven PAH whose bioaccumulation is represented by benzo(a)pyrene. In addition to reconsidering USEPA's application of an FCM to PAH, USEPA's framework and generally acknowledged scientific understanding of the parameters that affect bioaccumulation suggest that States should use State-specific data, if available, to develop State-specific DOC/POC concentrations and State-specific trophic level lipid contents, as well as considering the applicability to State waters and scientific basis of other aspects of USEPA's 2016 bioaccumulation methodology.

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ATTACHMENT G

Estimation of the Degree of Conservatism Implicit in Human Health Water Quality Criteria due to Not Considering Fish Exposure and Oceanic Dilution

Estimation of the Degree of Conservatism Implicit in Human Health Water Quality Criteria due to Not Considering Fish Exposure and Oceanic Dilution

NCASI

July 8, 2016

Summary

A procedure relating fish habitat and oceanic dilution to salinity is developed in order to estimate the degree of conservatism introduced by not considering dilution in the fish exposure calculations used to generate human health water quality criteria (HHWQC). Using lower boundary values of estuarine and marine salinities, this procedure estimates that the rate of fish exposure is overstated by 31-41% (depending upon the substance's BAF) by not considering oceanic dilution. Sensitivity analysis suggests that using more realistic, species specific, salinities to define estuarine habitat would add 10% or more to this estimate.

Background

The most recent version (FDEP 2016) of FDEP's technical support document for derivation of human health criteria indicates that risk is calculated by one of two equations depending upon the carcinogenicity of the evaluated compound.

For non-carcinogens:

$$HQ = \frac{I_W + I_F}{BW * RfD} \qquad \textit{Equation 1}$$

Where: HQ = Hazard Quotient
I_W = Drinking water exposure (mg/day)
I_F = Fish ingestion exposure (mg/day)
BW = Body weight (kg)
RfD = Reference dose (mg/kg day)

Carcinogens:

$$Risk = \frac{(I_W + I_F + D_S) * CSF}{BW} \qquad \textit{Equation 2}$$

Where: D_S = Dermal contact intake (mg/day)
CSF = Cancer slope factor (1/(mg/kg day))

Focusing on the fish consumption exposure route (I_F), the daily intake of a particular compound is estimated by:

$$I_F = \sum_{i=2}^{4} FCR_i * BAF_i * SWC \qquad \textit{Equation 3}$$

I_F = exposure through fish consumption (mg/day)
i = aquatic trophic level of fish species (2, 3, or 4)
SWC = surface water concentration (mg/L)
FCR_i = fish ingestion rate for aquatic trophic level *i* (gm/day)
BAF_i = bioaccumulation factor for aquatic trophic level *i* (L/day)

Equation 3 estimates the daily rate of exposure to a compound as a function of fish consumption from each of three aquatic trophic levels, the BAF for each trophic level and the concentration of the compound in surface waters. Note that BAF values unique to the aquatic trophic levels (which necessitates FCRs corresponding to those tropic levels) are a new feature of the latest TSD.

In equation 3, surface water concentration (*SWC*) of the compound is constant, implying that throughout the fresh water, estuarine, and near shore marine environs, no concentration change takes place (i.e. all species, regardless of habitat, would be exposed at the water quality criteria concentration). However, in a previous report, NCASI (2016) demonstrated that in at least two estuaries (and based on the prevailing science, it is expected that all estuaries would show similar traits) the *SWC* of a compound originating from the freshwater source would be diluted with ocean water (containing a negligible amount of the compound) as it entered and moved through an estuary system. Thus, species living in increasingly saline environments would be expected to be exposed at concentrations which would be increasingly diluted relative to the water quality criteria concentration. The assumption that *SWC* is constant throughout the estuary overstates the human exposure via the consumption of fish that spend most or all of their life histories in marine or estuarine environments.

Objective

Estimate the degree of conservatism introduced to the fish consumption exposure calculation by not accounting for oceanic dilution.

Methods

The basis for the following estimation calculations is the concept that in transitional freshwater/estuarine/marine systems, salinity can define both fish habitat and the degree of oceanic dilution. Fish typically stay within relatively narrow salinity ranges due to specific physiological adaptations required to survive in either a more or less saline environment. While juvenile fish species may migrate to a different salinity environment as they mature, adult species (which are most commonly taken as seafood) generally remain within the same salinity range for their remaining lifespan.

Salinity also can be used to calculate the extent of oceanic dilution occurring at a particular location. A transitional freshwater/estuarine/marine system has two major sources of water flow; the freshwater river and the saltwater ocean. Given that these water sources have a well-known (less than 0.5 ppt for

freshwater and about 35 ppt for ocean water) salinity, long term average mixing calculations using salt as a conservative tracer can provide the ratio of ocean water to freshwater at an intermediate location where salinity is known. Therefore, if a certain fish species only lives in salinities greater than 10 ppt, the oceanic dilution of the freshwater source at that 10 ppt location can be calculated. This dilution can then be applied to the exposure calculations via a dilution factor, *DF* (i.e. the ratio of a substance's concentration at the intermediate location to the concentration in the freshwater). The development of *DF* is presented in Appendix I and the incorporation of *DF* into the fish exposure calculation (Equation 3) is shown in Equation 4.

$$I_F = \sum_{i=2}^{4}\left[\sum_{j=1}^{3} FCR_{i,j} * SWC * DF_j\right] * BAF_i \qquad \textit{Equation 4}$$

Where i = aquatic trophic level 2, 3 or 4

j = salinity habitat, where 1 = freshwater, 2 = estuarine, 3 = marine

The remainder of this paper is a direct comparison of Equation 3 and Equation 4. The only difference between the equations is that Equation 4 includes a term (*DF*) that adjusts the exposure concentration (*SWC*) to account for oceanic dilution. Thus, the difference between Equations 3 and 4 is an estimation of the effect of *not considering oceanic dilution* when calculating fish consumption exposure.

Implementation of Equations 3 and 4

In order to implement Equations 3 and 4, several pieces of information are required to populate the variables with realistic values, including:

- Daily fish consumption information.
    - Total amount fish consumed.
    - Species of fish.
    - Fraction of each species consumed relative to the total consumption.
- The trophic level or levels to which each species is assigned.
- The BAF for each trophic level or levels for each species.
- The water concentration of the pollutant of concern, assumed in this example to be 1 mg/L in freshwater and 0.01 mg/L in ocean water.

The source of information for the above requirements is FDEP's most recent technical support document (FDEP 2016). The fraction of each species consumed was back-calculated from the data provided in Table 3.5. In addition to the information required for Equation 3, Equation 4 also needs each species to be apportioned to a salinity habitat. This was done using EPA's Habitat Apportionment Document (EPA 2016) to assign each fish species to freshwater, estuarine or marine (or some combination of two). Salinity definitions of these habitats were based upon the USGS (2016) where freshwater is < 0.5 ppt, estuarine: 0.5 – 25 ppt, and marine: > 25 ppt. Because it was recognized that the salinity definitions provided by USGS may not match with most species actual salinity preference (i.e. a salinity of 0.5 ppt may be classified as "estuarine" but many estuarine adult species require significantly

higher salinity), this is considered a rough, likely conservative, approximation. In order to understand the sensitivity of the estimate to the estuarine salinity definition, Equation 4 was also evaluated using an estuarine salinity of 8.5 ppt, which is the lower range of the most freshwater tolerant Florida shrimp species; brown shrimp (USFWS 1989).

Results

Fish exposure rates (mg/day) were calculated for a selection of different compounds with varying BAFs using Equation 3, Equation 4 with the USGS definition of estuarine salinity and Equation 4 using the brown shrimp salinity preference as the definition of estuarine salinity conditions. The results are presented in Table 1 for randomly selected compounds in order of highest to lowest BAF along with the percent difference between Equation 3 and Equation 4.

Table 1. Fish Exposure Rates (mg/kg) and Percent Difference for a Selection of Compounds Calculated by Equations 3 and 4

Compound (Trophic Level 4 BAF, L/kg)	Equation 3	Equation 4 (Estuarine Salinity @ 0.5 ppt)	Equation 4 (Estuarine Salinity @ 8.5 ppt)
4,4'-DDT (390000)	4196	2462 (41%)	2198 (48%)
Aldrin (240000)	2953	1800 (39%)	1601 (46%)
Toxaphene (3900)	68.0	45 (34%)	39.2 (42%)
Vinyl Chloride(1.5)	0.031	0.021 (31%)	0.018 (41%)

These results suggest that not considering oceanic dilution in the fish exposure calculation of HHWQC can lead to significant over-estimation of the actual exposure. This overestimate ranges from 30% to nearly 50% in the above example. However, the sensitivity analysis of estuarine salinity suggests that this value is likely higher due to conservative assumptions regarding habitat for the fish species:

- Brown shrimp (used to define estuarine salinity in Table 1) are the most freshwater tolerant of the major Florida shrimp species, adult white and pink shrimp prefer salinities greater than 25 ppt.
- Some species classified as marine (i.e. adult red snapper), prefer salinities higher than the USGS definition of marine salinity.
- The oceanic concentration of pollutant was assumed to be 100x less than the freshwater concentration; however it is likely in many cases much less.

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Appendix I. Derivation of Dilution Factor

If two sources (1 and 2) of water are mixing, the concentration and flow at any point (3) are defined by the boundary concentrations and relative flow contribution via materials balance:

$$Q_1 s_1 + Q_2 s_2 - Q_3 s_3 = 0 \qquad \text{Equation A1}$$

$$Q_1 + Q_2 - Q_3 = 0 \qquad \text{Equation A2}$$

Where: Q = flow (V/T)
s = salinity (M/V)
subscript 1 = denotes upstream "freshwater" location boundary
subscript 2 = denotes downstream "oceanic" location boundary
subscript 3 = denotes location of interest

Rearranging and substituting (A2) into (A1) gives (A3):

$$Q_1 s_1 + Q_2 s_2 = (Q_1 + Q_2) s_3 \qquad \text{Equation A3}$$

If the boundary salinities s_1 and s_2 and the salinity at position 3 in the estuary are known, the flow ratio (Q_1/Q_2) at position 3 can be derived:

$$\frac{Q_1}{Q_2} = \frac{s_3 - s_2}{s_1 - s_3} \qquad \text{Equation A4}$$

To calculate the concentration of a substance other than salt at position 3, new boundary conditions (p_1 and p_2) must be established, but the flow ratio calculated using salinity remains constant for that position. Substituting *p* for *s* to denote a new substance and algebraically solving for p_3 in Equation A4 yields:

$$p_3 = \frac{-p_2 - \frac{Q_1}{Q_2} p_1}{-\frac{Q_1}{Q_2} - 1} \qquad \text{Equation A5}$$

A dilution factor, *DF* (i.e. the ratio of the substance concentration at position 3 to the concentration in the freshwaters) p_3/p_1, can be calculated by rearranging the terms in (A5).

$$\frac{p_3}{p_1} = \frac{-p_2}{\left(-\frac{Q_1}{Q_2} - 1\right) * p_1} - \frac{\frac{Q_1}{Q_2}}{\frac{-Q_1}{Q_2} - 1} \qquad \text{Equation A6}$$

ATTACHMENT H

A Review of Methods for Deriving Human Health-Based Water Quality Criteria with Consideration of Protectiveness

A REVIEW OF METHODS FOR DERIVING HUMAN HEALTH-BASED WATER QUALITY CRITERIA WITH CONSIDERATION OF PROTECTIVENESS

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National Council for Air and Stream Improvement

CONTENTS

APPENDICES

TABLES

AN OVERVIEW OF PARAMETERS USED IN THE DERIVATION OF EPA HUMAN HEALTH AMBIENT WATER QUALITY CRITERIA

1.0 EXECUTIVE SUMMARY

Consistent with the requirements of the Clean Water Act, states are obligated to establish numeric water quality criteria for toxic substances and to periodically consider the need for revisions to those criteria. Toxics criteria are designed to protect both resident aquatic life and humans exposed via drinking water, consumption of fish, and/or dermal contact. Criteria for the protection of human health (i.e., Human Health Ambient Water Quality Criteria, or HHAWQC) are traditionally derived using EPA-recommended equations that include parameters for risk, toxicity, and exposure. The values used for these parameters are revisited and adjusted periodically in response to the availability of new science and shifts in policy.

The material presented in this paper includes an overview of the derivation procedures for HHAWQC, focusing especially on the selection of values for the parametric components in the HHAWQC derivation equations. Particular attention is given to the use of conservative (i.e., over-protective) choices for multiple parameter values and the overall effect of compounded conservatism on the resulting criteria relative to health protection targets established by state and federal agencies.

1.1 Parameters Used in HHAWQC Derivation and Frequently Used Values

The equations used to derive HHAWQC are composed of explicit parameters (i.e., those that are listed and defined), and implicit parameters (i.e., those that are embodied with the application of the explicit parameters). The equations and rationales for selection of specific parameter values were developed by EPA more than twenty years ago and while updates in parameter values have been made periodically, the basic methodology remains unchanged. **Table 1.1** lists the explicit and implicit parameters used in the HHAWQC derivation. Also shown are typical parameter values recommended by EPA. The third column in the table provides an indication regarding whether the typical value reflects a central, upper-end, or maximum in the range of values that could be chosen for each parameter. It is clear from the table that, in nearly every case, the typical values used for explicit and implicit parameters are selected from the upper end of the range of possible values.

It is well-known, and mathematically intuitive, that the practice of selecting "upper end of range" values for multiple parameters in a risk equation will lead to over-conservative estimates of risk or, in the case of HHAWQC, overly restrictive criteria. Indeed, EPA's Risk Assessment Task Force has suggested that "when several parameters are assessed, upper-end values and/or central tendency values are generally combined to generate a risk estimate that falls within the higher end of the population risk range" and "an exposure estimate that lies between the 90^{th} percentile and the maximum exposure in the exposed population [should] be constructed by using maximum or near-maximum values for one or more of the most sensitive variables, leaving others at their mean values" (EPA 2004). This concept, however, has not been embraced in the current practice for deriving HHAWQC.

Table 1.1 Parameter Values used in HHAWQC Derivation and Location in the Range of Possible Values

Parameter	Typical Value	Location in Range of Possible Values[1] (maximum possible, upper-end, or central tendency)
Explicit Parameters		
substance toxicity	substance-specific	upper-end
body weight of a person	70 kg (actual mean is 80kg)	central tendency
drinking water intake	2 L/day (86th percentile), but assumes drinking water is untreated surface water	(extreme) upper-end
fish ingestion/consumption rate	17.5 g/day (90th percentile of sport fishers)	upper-end
substance exposure from other sources	80%	upper-end
Implicit Parameters		
cooking loss	0% (no loss due to cooking)	maximum possible
duration of exposure	70 years	(extreme) upper end
exposure concentration	at HHAWQC 100% of the time	maximum possible
relative bioavailability	1	maximum possible
bioaccumulation/concentration factor of fish	substance-specific	substance-specific (not evaluated)

[1]"maximum possible" would be the most conservative (over protective) choice possible, "upper-end" a very conservative choice, and "central tendency" a typical or average value for a population. "Extreme" denotes a value that is very near maximum.

1.2 Degree of Conservatism in HHAWQC

Section 6 of this report details the degree of protectiveness, conservatism, and the combined effect of conservative parameter value choices in the derivation of HHAWQC. The information provided shows that the values commonly used for each parameter can have the effect of lowering the calculated HHAWQC by large factors. For example:

- substance toxicity values are commonly reduced by 10 to 3000 times below demonstrated toxicity thresholds as a means of ensuring protection of human health
- assumptions about chemical exposure via drinking water results in some criteria being as much as 30 times lower than needed to afford the degree of protection targeted by most states and EPA

- the assumption that a person lives in the same place and is exposed to the same level of contamination for a 70 year lifetime results in criteria that are up to 8 times more stringent than if a median exposure period were assumed
- the assumption that waters would exist at the allowable HHAWQC for 70 years is in opposition to water management policies in virtually all states and results in criteria values that are 1.5 to 6 times more stringent than would be the case if actual water quality management practices were considered

Each of the factors listed above, and several others discussed in more detail in the following sections, can combine (i.e., compound) when applied in the same calculation, such as that used for deriving HHAWQC. The result is criteria that are many times lower than would be the case if the advice of the Risk Assessment Task Force regarding use of upper range values for one or more sensitive values and leaving others at their mean values (EPA 2004) were followed.

1.3 Comparison of HHAWQC with other Regulatory Mechanisms for Human Health Protection

The summary above, and supporting sections of this report, offer observations suggesting that HHAWQC are considerably more protective (i.e., lower in concentration, or over-protective) than are necessary to achieve the health protection targets described by EPA and many state environmental agencies. Section 7 of this report considers other evidence that might confirm or refute this observation. It contains a comparison of fish tissue concentrations corresponding to EPA recommended HHAWQC with (a) existing fish tissue concentration data, (b) concentrations found in other foods, and (c) allowable concentrations (such as fish consumption advisory "trigger levels") set by other US and international health agencies.

Findings from this comparison support the observation that HHAWQC are over-protective. Specifically:

- For higher assumed fish consumption rates and based on EPA fish tissue data, virtually all surface waters in the US would exceed the HHAWQC for PCB, mercury, and likely a number of other substances. In contrast, for example, health agencies have established fish consumption advisories for PCBs on only about 15% of water bodies (Appendix C) indicating that assumptions used by EPA are more conservative than the assumptions used by state agencies to derive fish consumption advisories.
- A comparison of the daily intake of several example substances for which HHAWQC exist, showed that intakes from other foodstuffs was greater than from fish and was already exceeding the allowable intakes used to establish HHAWQC. Thus, establishment and enforcement of more stringent HHAWQC may not provide a measureable public health benefit.
- Various federal and international agencies have established concentration limits for fish as a food in commerce. Levels set by these agencies (whose goal is to insure the safety of edible fish) show that EPA HHAWQC are limiting fish tissue concentrations to levels substantially (10s to 1000s of times) below those considered to be without significant risk.

1.4 Other Observations

Other observations from this review are noted as follows.

- Target cancer risk levels between 10^{-6} and 10^{-4} have become widely accepted among the different EPA programs, including the derivation of HHAWQC. The HHAWQC methodology document states that a risk level of 10^{-4} for highly exposed populations is acceptable (EPA 2000a). This is sometimes interpreted as meaning that highly exposed

populations are not as well protected by the HHAWQC. However, as noted by Kocher (1996) "if only a small population would be at greatest risk, the expected number of excess cancers corresponding to individual risks at the *de minimis* level of 10^{-4} would still be [essentially] zero."

- The fish consumption rates used in calculating HHAWQC can have a significant impact on the resulting HHAWQC. This is because the HHAWQC are proportional to the fish consumption rates - as the rate increases, the HHAWQC decreases, and the decrease is particularly pronounced for high BAF/BCF substances. Potential exposure through the fish consumption pathway is dependent upon a number of different variables including the types of fish consumed, the sources of those fish (particularly anadromous fish such as salmon, see Appendix B), and the rates at which they are consumed, all of which vary widely among the population. The quantification of fish consumption rates is complicated by the methods used to collect consumption information, the interpretation of such data (particularly extremes in the distribution of individual consumption rates obtained from survey data), the availability of fish from regulated sources, and the habits of the targeted population of fish consumers. Without extreme diligence in data interpretation, most of these complications are likely to manifest in overestimations of fish consumption rates.

- The selection of some exposure parameters are unrealistic because, as a practical matter, other environmental management programs would ensure that such conditions did not occur (or would not persist for a person's lifetime). Assumptions concerning ambient water column concentrations (and related fish tissue concentrations) and drinking water concentrations are examples.

Finally, it is noteworthy that the values used for parameters in a health risk equation like that for deriving HHAWQC involve a combination of science and policy choices. And, while evolving science and policy may sometimes indicate that revisiting these choices is warranted, responsible evaluation of risk (and thus protection of health) is best considered in total rather than by simple alteration of a single parameter value without due consideration of the others. The information presented herein suggests that the degree of protection embodied in the current HHAWQC derivation method, using typically applied values for each parameter, exceeds by a large margin the health protection targets expressed by EPA and many states.

2.0 INTRODUCTION

Section 304(a) (1) of the Clean Water Act (CWA) requires the United States Environmental Protection Agency (EPA) to develop and publish recommended numeric ambient water quality criteria (AWQC) for limiting the impact of pollutants on human health and aquatic life. These recommended human health-based AWQC (HHAWQC) are intended to provide guidance for states and tribes to use in adopting their own water quality standards and are meant to "minimize the risk of adverse effects occurring to humans from chronic (lifetime) exposures to substances through the ingestion of drinking water and consumption of fish obtained from surface waters" (EPA 2000a). Water quality criteria recommendations are derived by EPA using equations that express a risk analysis. The value of each parametric component of the criteria equations represents policy choices made by the Agency, though several of those choices are derived from scientific data (EPA 2011a).

In a staff policy paper from the Office of the Science Advisor, EPA discussed the bases for these policy choices (EPA, 2004). They noted that "Congress establishes legal requirements that generally describe the level of protectiveness that EPA regulations must achieve" and that individual statutes identify the risks that should be evaluated and protected against and also mandate the required levels of protection (EPA 2004). The Clean Water Act, which mandates the development of AWQC, simply

requires that AWQC must "protect the public health or welfare, enhance the quality of water and serve the purposes of this Act" and "be adequate to protect public health and the environment from any reasonably anticipated adverse effects of each pollutant." In order to meet these requirements, EPA "attempts to protect individuals who represent high-end exposures (typically around the 90th percentile and above) or those who have some underlying biological sensitivity" (but not hypersensitive individuals) (EPA 2004). EPA (2004) notes that "[p]rograms may approach the problem semi-quantitatively (e.g., selecting individual parameter values at specified percentiles of a distribution) or qualitatively (e.g., making conservative assumptions to ensure protection for most individuals), though no overall degree of protection can be explicitly stated."

While EPA is obligated to develop and publish AWQC guidance, adoption and implementation of criteria for most fresh waters in the U.S. is an activity mandated to states. Many states choose to adopt EPA's AWQC guidance values but states are free to depart from EPA's criteria guidance provided that there is a scientifically valid rationale for doing so. Departure from the EPA AWQC guidance values is commonly accomplished by altering one or more of the values used to represent the parametric components of the risk analysis equation used to derive the criteria guidance values.

This document contains a discussion of each parametric component of the risk analysis equation that is used to derive HHAWQC. As noted earlier, selection of parameter values for risk analyses is primarily a policy choice and it is typical that such choices are conservative in favor of protecting public health. The combined degree of conservatism embodied in the final AWQC guidance is not usually expressed quantitatively by EPA. The primary purpose of this document is to provide an exploration of the combined conservatism that may be embodied in AWQC calculated using typically chosen values for the explicit parametric components of the HHAWQC equation and use of implicit assumptions also embodied in the criteria derivation.

3.0 EQUATIONS USED FOR THE DERIVATION OF HHAWQC

In calculating HHAWQC, EPA differentiates between carcinogenic and noncarcinogenic effects. Three risk analysis equations are used, the first for noncarcinogenic effects, the second for carcinogenic effects that are assumed to have a nonlinear dose-response, and the third for carcinogenic effects that are assumed to have a linear dose-response. These are shown in Table 3.1.

Table 3.1 Equations for Deriving Human Health Water Quality Criteria

Substance Category	HHAWQC Equation	Eq. #
Noncarcinogenic effects	$RfD*RSC*(BW/(DI + (\Sigma FI_i*BAF_i)))$	**Eq. 3.1**
Carcinogenic effects (non-linear)	$(POD/UF)*RSC*(BW/(DI + (\Sigma FI_i*BAF_i)))$	**Eq. 3.2**
Carcinogenic effects (linear)	$RSD*(BW/(DI + (\Sigma FI_i*BAF_i)))$	**Eq. 3.3**

where:

HHAWQC = human health ambient water quality criterion (mg/L);

RfD = reference dose for noncancer effect (mg/kg-day);

RSC = relative source contribution factor to account for non-water sources of exposure (typically expressed as a fraction of the total exposure);

POD = point of departure for carcinogenic effects based on a nonlinear low-dose extrapolation (mg/kg-day), usually a LOAEL, NOAEL, or LED_{10};

UF = uncertainty factor for carcinogenic effects based on a nonlinear low-dose extrapolation (unitless);

RSD = Risk-specific dose for carcinogenic effects based on a linear low-dose extrapolation (mg/kg-day) and on the selected target risk level;

BW = human body weight (kg);

DI = drinking water intake (L/day);

FI_i = fish intake at trophic level (TL) i (i = 2, 3, and 4); this is the fish consumption rate (kg/d); and

BAF_i = bioaccumulation factor at trophic level i, lipid normalized (L/kg)

The first portion of each equation in Table 3.1 contains parameters that represent a measure of the toxicity of a substance and are unique to each equation. The latter portion of each equation is common for the three substance categories and describes assumed human exposure to a substance. Implicit, and not obvious, with the practice of using these equations are other assumptions concerning exposure (i.e., a duration of exposure equal to a full lifetime, an average ambient water concentration equal to the HHAWQC, and bioavailability of chemicals from fish and water equal to that observed in the toxicity experiment). Finally, and also not obvious, is that an assumed incremental risk of illness is also part of the overall algorithms. Taken collectively, these explicit and implicit elements yield a risk analysis in the form of an acceptable water column concentration for a substance.

Although the parameters in the risk equations used for deriving a HHAWQC are most accurately represented by a range or distribution of values, it has been typical for EPA to select a single value for each parameter. EPA has recognized that there are elements of both variability and uncertainty in each parametric value but has generally not implemented specific procedures to account for variability and uncertainty. However in some cases, EPA has intentionally chosen parametric values that are conservative (i.e., over-, rather than under-, protective of human health) with respect to the general population.

The sections below discuss the parametric components of the toxicity portion (Section 4) and the exposure portion (Section 5) of each equation in Table 3.1. Section 6 includes discussion of variability and uncertainty in parameter values and, where evident, conservatism embodied in typical choices made for parameter values. Also in Section 6, consideration is given to the combined effect on conservatism of typical parameter value choices in HHAWQC derivation.

4.0 TOXICITY PARAMETERS USED FOR DERIVATION OF HHAWQC

Each of the three equations used to develop HHAWQC contains a factor that represents the toxicity of the substance of concern. Equation 3.1 (Table 3.1), which is used for non-carcinogenic effects, employs the reference dose (RfD), the derivation of which incorporates various uncertainty factors (UFs) and sometimes an additional modifying factor (MF). Equation 3.2 (Table 3.1), which is used for carcinogenic effects that have a nonlinear dose-response curve (i.e., there exists some level of exposure below which no carcinogenic response is expected to occur), employs a factor calculated by dividing the "point of departure" (POD) by UFs. Equation 3.3 (Table 3.1), which is used for substances that are assumed to have a linear dose-response (i.e., some probability of a carcinogenic response is presumed to exist at any level of exposure), employs a Risk-Specific Dose (RSD). It is EPA's policy to assume that all carcinogenic effects can be described using a linear dose response

unless non-linearity has been clearly demonstrated. Typically, if a compound is considered to have both carcinogenic and non-carcinogenic health effects, HHAWQC are calculated for both the cancer and noncancer endpoints and the lower of the two concentrations is selected as the HHAWQC. The derivation of these components is described in the "Methodology for Deriving Ambient Water Quality Criteria for the Protection of Human Health (EPA 2000a) (hereafter referred to as the "HHAWQC methodology document") and its Technical Support Document Volume 1: Risk Assessment" (EPA 2000b).

4.1 Reference Dose (RfD)

A reference dose (RfD) is defined as "an estimate (with uncertainty spanning approximately an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious effects over a lifetime" (EPA 2000b).

The development of an RfD begins with a review of all available toxicological data. Relevant studies are evaluated for quality and a "critical effect" is identified. The critical effect is defined as "the first adverse effect, or its known precursor, that occurs to the most sensitive species as the dose rate of an agent increases" (EPA 2002a). The underlying assumption is that if the RfD is derived to prevent the critical effect from occurring, then no other effects of concern will occur (EPA 2002a).

The next step is the identification of a POD based on the study in which the selected critical effect has been identified. The POD may be derived from a No Observed Adverse Effect Level (NOAEL), a Lowest Observed Adverse Effect Level (LOAEL) or Benchmark Dose Lower Confidence Level (BMDL). The NOAEL is defined by USEPA as "the highest exposure level at which there are no biologically significant increases in the frequency or severity of an adverse effect between the exposed population and its appropriate control; some effects may be produced at this level, but they are not considered adverse or precursors of adverse effects."[1] If a NOAEL cannot be identified, a LOAEL may be used instead. The LOAEL is defined by USEPA as "the lowest exposure level at which there are biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group."[2]

When study data are suitable, the Benchmark Dose BMD approach is sometimes used as an alternative to the NOAEL/LOAEL approach. The BMD is the dose at which the critical effect occurs at a rate 5-10% above the rate observed in the control group (other rates could possibly be used, but 5% or 10% are most common). The BMDL, which is typically the lower 95% confidence limit of the BMD, is used as the POD when the BMD approach is used.

Once the POD is identified, the RfD is derived according to equation 4.1:

$$RfD = POD/(UF_i * MF) \qquad \textbf{Eq. 4.1}$$

where:

RfD = reference dose for noncancer effect (mg/kg-day);

POD = NOAEL, LOAEL, or BMDL (mg/kg-day);

UF_i = uncertainty factors for various circumstances (see Table 4.1) (unitless) ; and

MF = modifying factor (unitless)

[1] Taken from USEPA's online IRIS glossary (http://www.epa.gov/iris/help_gloss.htm#n)
[2] Taken from USEPA's online IRIS glossary (http://www.epa.gov/iris/help_gloss.htm#n)

Uncertainty factors are used to reduce the dose in order to account for areas of scientific uncertainty in the supporting toxicity databases (EPA 2000b). The standard UFs are 1, 3, and 10. A modifying factor further adjusts the dose in order to provide for additional uncertainty not explicitly included in the UFs, such as the completeness of the overall database (EPA 2000b). The MF is a matter of professional judgment and ranges between 0 and 10, with the standard values being 0.3, 1, 3, and 10 and the default value being 1 (EPA 2000b). Table 4.1 defines the various UFs.

Table 4.1 Uncertainty Factors (adapted from EPA 2000b)

Uncertainty Factor	Description
Intraspecies variation (UF_H)	Accounts for uncertainty associated with variations in sensitivity among members of the same species (e.g., differences in age, disease status, susceptibility to disease due to genetic differences)
Interspecies variation (UF_A)	Accounts for uncertainty involved in extrapolating from animal data to humans; used when the POD is derived from an animal study
Subchronic-to-chronic (UF_S)	Accounts for uncertainty involved in extrapolating from studies with a less-than-chronic[1] duration of exposure; used when the POD is derived from a study in which exposures did not occur over a significant fraction of the animal's or the individual's lifetime
LOAEL-to-NOAEL (UF_L)	Accounts for uncertainty associated with the use of a POD derived from a LOAEL rather than a NOAEL or BMDL
Incomplete database (UF_D)	Accounts for uncertainty associated with the use of an incomplete database to derive the POD, for example, the lack of a study of reproductive toxicity

[1] Chronic Exposure: Repeated exposure for more than approximately 10% of the life span in humans (more than approximately 90 days to 2 years in typically used laboratory animal species).

In application, the various UFs and any MF are multiplied to obtain the final factor by which the POD is to be divided. In general, EPA follows a policy that a final factor greater than 3000 indicates that the existing toxicity database is inadequate to support the derivation of an RfD. In this case, no RfD is calculated (EPA 2002a).

Although instructions for calculating an RfD are provided in the documentation for HHAWQC, in actual practice, the RfD is typically obtained from EPA's IRIS database (http://www.epa.gov/iris/).

4.2 Cancer Effects: Nonlinear Low-Dose Extrapolation

In deriving a HHAWQC, a nonlinear low-dose extrapolation may be used for carcinogenic effects when there are sufficient data available to understand the mode of action (MOA) and conclude that it is nonlinear at low doses (EPA 2005). In practical application, this is interpreted to mean that a threshold of exposure exists below which no carcinogenic response will occur.

For nonlinear carcinogenic effects, the factor representing toxicity in Equation 3.2 is calculated by dividing the POD by UFs. The recommended POD is the Lower Limit on Effective $Dose_{10}$, or LED_{10}, which is determined by calculating the lower 95 percent confidence limit on a dose associated with an estimated 10 percent increased tumor or tumor precursor response (EPA 2000b). A NOAEL or LOAEL value from a precursor response may also be used in some cases (EPA 2000b). When animal data are used to determine the POD, the selected dose is converted to a human equivalent dose using a default interspecies dose adjustment factor or a toxicokinetic model. However, as noted above, it is EPA's policy to assume that all carcinogenic effects have a linear dose response unless non-linearity has been clearly demonstrated. Thus, the non-linear low dose extrapolation procedure is rarely used.

The HHAWQC methodology document provides no specific guidance on the selection of UFs (EPA 2000a). Instead, it defers to the "upcoming cancer risk assessment guidelines," which were subsequently released in 2005.

The 2005 Cancer Risk Assessment Guidelines took a somewhat different approach than anticipated by EPA in 2000 when the HHAWQC methodology guidelines were developed. The 2005 guidelines instead recommended that for nonlinear carcinogenic effects, "an oral reference dose…should be developed in accordance with EPA's established practice for developing such values" (EPA 2005). This does not have much practical impact on HHAWQC calculation, as comparison of equations 3.2 and 4.1 reveals that the process for calculating the factor that represents the toxicity of nonlinear carcinogenic effects in HHAWQC derivations is essentially the same as that for calculating an RfD.

Given that (1) the documentation for HHAWQC derivation does not provide complete guidance on the calculation of the POD/UF factor, and (2) the 2005 Cancer Risk Assessment Guidelines took a somewhat different approach than anticipated by the HHAWQC methodology guidelines, in actual practice, the POD/UF factor will be typically be replaced by an RfD for some noncancer endpoint (e.g., a cancer precursor event) obtained from EPA's IRIS database (http://www.epa.gov/iris/).

4.3 Cancer Effects: Linear Low-Dose Extrapolation

In deriving a HHAWQC, a linear low-dose extrapolation is used for compounds that are believed to have carcinogenic potential when the chemical has direct effects on DNA, the MOA analysis indicates that the dose-response relationship will be linear, human exposures or body burdens are already near the doses associated with key events in the carcinogenic process, or there is an absence of sufficient data to elucidate the MOA.

The RSD, which is used in Equation 3.3 (Table 3.1), is derived according to Equation 4.2:

$$\text{RSD} = \text{Target Incremental Cancer Risk}/m \qquad \textbf{Eq. 4.2}$$

where:

RSD = Risk-Specific dose (mg/kg-day);

Target Incremental Cancer Risk = Typically a value ranging from 10^{-6} to 10^{-4}; and

m = cancer potency factor $(\text{mg/kg-day})^{-1}$

The HHAWQC methodology document (EPA 2000a) states that the Agency will calculate recommended HHAWQC using at a Target Incremental Cancer Risk level of 10^{-6}. However, in deriving their own HHAWQC, states and authorized tribes may choose a risk level as low as 10^{-7} or as high as 10^{-5}, as long as the risk to more highly exposed subgroups (e.g., sport or subsistence anglers) does not exceed 10^{-4}. (The rationale for this is discussed further in Section 6.1.3.)

The cancer potency factor may be calculated by first modeling the relationship between tumor incidence and dose and then selecting a POD (generally the LED_{10}). When animal data are used to

determine the POD, the selected dose is converted to a human equivalent dose using a default interspecies dose adjustment factor or a toxicokinetic model. Finally, a straight line is drawn between the POD and the origin (zero). The slope of that line, which will be "m" in Equation 4.2, is calculated. If the LED_{10} is used as the POD, m is equal to $0.10/LED_{10}$ (EPA 2000b).

Instructions for calculating m are provided in the documentation for HHAWQC. In actual practice, however, the value of m is typically obtained from EPA's IRIS database (http://www.epa.gov/iris/). Note that EPA terminology has changed somewhat since the HHAWQC methodology document was released and what was referred to as "m" or "cancer potency factor" in the methodology document is more commonly identified as "slope factor" in the IRIS database.

5.0 EXPOSURE PARAMETERS USED FOR DERIVATION OF HHAWQC

As noted above, both explicit and implicit elements are used to yield a risk analysis in the form of an acceptable water column concentration for a substance. This section summarizes each of these elements and the manner in which they are used for deriving HHAWQC.

5.1 Relative Source Contribution (RSC)

When deriving a HHAWQC for noncarcinogenic or nonlinear carcinogenic effects, a factor is included in the equation to account for non-water sources of exposure to a substance. For example, a particular chemical may be found not only in water sources, but also in some food items or in ambient air (from which it could be inhaled). This factor is known as the Relative Source Contribution (RSC) and it acts to reduce the amount of the RfD that is apportioned to water and fish consumption. The rationale for using the RSC factor in calculating a HHAWQC is to ensure that an individual's total exposure does not exceed the threshold level (EPA 2000a).

The HHAWQC methodology document (EPA 2000a) creates an "Exposure Decision Tree" procedure to be used in the selection of an RSC. In the absence of sufficient data to support the use of the Exposure Decision Tree, EPA uses 20% as a default RSC (EPA 2000a). The methodology also sets 80% as the maximum allowable RSC and 20% as the minimum (EPA 2000a). EPA encourages states and authorized tribes to develop alternate RSC values based on local data (EPA 2000a). Although the Exposure Decision Tree approach does theoretically allow for the use of an RSC other than the 20% default, in actual practice, use of values other than the default is very rare.

Note that while the methodology (EPA 2000a) specifies that the RSC value must be between 20 and 80% and states that "EPA intends to use 20 percent of the RfD (or POD/UF), which has also been used in past water program regulations, as the default value," the current EPA HHAWQC are calculated using RSCs ranging from 20 to 100%. This is because many of the HHAWQC remain unchanged from earlier years or have been updated to reflect changes in fish consumption rates or RfD, but were not recalculated using the 2000 methodology.

The RSC factor is not used in the derivation of HHAWQC for carcinogenic effects with linear low-dose extrapolation. For these substances, the only sources considered are drinking water and fish ingestion. This is because for these substances, the HHAWQC is being determined with respect to the *incremental* lifetime risk posed by a substance's presence in water, and is not being set with regard to an individual's total risk from all sources of exposure (EPA 2000a). Thus, the HHAWQC for any substance represents the concentration of that substance in water that would be expected to increase an individual's lifetime cancer risk by no more than the target risk level, regardless of any additional lifetime cancer risk contributed by potential exposures from other sources (EPA 2000a).

5.2 Body Weight (BW)

The HHAWQC methodology document (EPA 2000a) recommends using a default body weight of 70 kg for calculating HHAWQC. This is considered to be a representative average body weight for male and female adults, combined. Adult values are used because the HHAWQC are intended to be protective over the full lifespan. The methodology also notes that 70 kg is used in the derivation of cancer slope factors and unit risks that appear in IRIS and advocates maintaining consistency between the dose-response relationship and exposure factors (EPA 2000a).

5.3 Drinking Water Intake (DI)

EPA recommends using a default drinking water intake rate of 2 L/day, which is believed to represent a majority of the population over the course of a lifetime (EPA 2000a).

The basis for the drinking water intake rate is the 1994-96 Continuing Survey of Food Intake by Individuals *(*CSFII) conducted by the U.S. Department of Agriculture (EPA 2000a). The CSFII survey collected dietary intake information from nationally representative samples of non-institutionalized persons residing in United States households (EPA 2000a). Households in these national surveys were sampled from the 50 states and the District of Columbia (EPA 2000a). Each survey collected daily consumption records for approximately 10,000 food codes across nine food groups (EPA 2000a). This included the number of fluid ounces of plain drinking water consumed and also information on the household source of plain drinking water, water used to prepare beverages, and water added during food preparation (EPA 2000a).

The results of the 1994-96 CSFII analysis indicated that the arithmetic mean, 75th, and 90th percentile values for adults 20 years and older were 1.1, 1.5, and 2.2 L/day, respectively (EPA 2000a). The 2 L/day value selected by EPA represents the 86^{th} percentile for adults (EPA 2000a).

5.4 Fish Ingestion Rate (FI)

Because the level of fish intake in highly exposed populations varies by geographical location, EPA suggests a four preference hierarchy for states and authorized tribes to follow when deriving consumption rates that encourages use of the best local, state, or regional data available (EPA 2000a). The four preference hierarchy is: (1) use of local data; (2) use of data reflecting similar geography/population groups; (3) use of data from national surveys; and (4) use of EPA's default intake rates (EPA 2000a).

EPA's first preference is that states and authorized tribes use the results from fish intake surveys of local watersheds within the state or tribal jurisdiction to establish fish intake rates that are representative of the defined populations being addressed for the particular waterbody (EPA 2000a). EPA also recommends that the fish consumption rate used to develop the HHAWQC be based only on consumption of freshwater/estuarine species (EPA 2000a). In addition, for noncarcinogens and nonlinear carcinogens, any consumption of marine species of fish should be accounted for in the calculation of the RSC (EPA 2000a). States and authorized tribes may use either high-end values (such as the 90th or 95th percentile values) or average values for the population that they plan to protect (e.g., subsistence fishers, sport fishers, or the general population) (EPA 2000a).

If surveys conducted in the geographic area of the state or tribe are not available, EPA's second preference is that states and authorized tribes consider results from existing fish intake surveys that reflect similar geography and population groups (e.g., from a neighboring state or tribe or a similar watershed type) (EPA 2000a). As with the use of fish intake surveys of local watersheds, consumption rates based on data collected from similar geographic and population groups should be based only on consumption of freshwater/estuarine species with any consumption of marine species accounted for in the calculation of the RSC (EPA 2000a).

If applicable consumption rates are not available from local, state, or regional surveys, EPA's third preference is that states and authorized tribes select intake rate assumptions for different population groups from national food consumption surveys (EPA 2000a). The HHAWQC methodology document (EPA 2000a) references a document titled "Estimated Per Capita Fish Consumption in the United States" (EPA 2000c) as the source for this information, however, there is a more recent document, "Exposure Factors Handbook: 2011 Edition" (EPA 2011b) that provides more current regional and subpopulation data and is also useful for this purpose. Again, EPA recommends that fish consumption rates be based on consumption of freshwater and estuarine species only and any consumption of marine species of fish should be accounted for in the calculation of the RSC (EPA 2000a).

As their fourth and last preference, EPA recommends the use of a default fish consumption value for the general adult population of 17.5 grams/day (EPA 2000a). This default value is used by EPA in its derivation of HHAWQC. This represents an estimate of the 90th percentile per capita consumption rate for the U.S. adult population based on the CSFII 1994-96 data (EPA 2000a). EPA believes that this default value will be protective of the majority of the general population (EPA 2000a). If a state or authorized tribe identifies specific populations of sportfishers or subsistence fishers that may represent more highly exposed individuals, EPA recommends default fish consumption rates of 17.5 grams/day and 142.4 grams/day, respectively, though in such cases a subpopulation risk level may also be appropriate (EPA 2000a) as explained in Section 6.1.3.

5.5 Bioaccumulation Factors (BAF) and Trophic Level

Bioaccumulation is the process in which aquatic organisms accumulate certain chemicals in their tissues when exposed to those chemicals through water, their diet, and other sources, such as sediments. In order to account for potential exposures to these chemicals through the consumption of fish and shellfish, EPA uses national bioaccumulation factors (BAFs) in the derivation of HHAWQC. The HHAWQC methodology document (EPA 2000a) defines BAF as the ratio (in L/kg tissue) of a concentration of a chemical in the tissues of commonly consumed aquatic organisms to its concentration in the surrounding water in situations where the organisms and their food are exposed and the ratio does not change substantially over time (i.e., the ratio which reflects bioaccumulation at or near steady-state).

The HHAWQC methodology document (EPA 2000a), the "Technical Support Document Volume 2: Development of National Bioaccumulation Factors" (EPA 2003a), and the "Technical Support Document Volume 3: Development of Site-Specific Bioaccumulation Factors" (EPA 2009) describe procedures for deriving national and site-specific BAFs. Separate procedures are provided for different types of chemicals (i.e., nonionic organic, ionic organic, inorganic and organometallic) (EPA 2000a). Also, EPA states that national BAFs should be derived separately for each trophic level because the concentrations of certain chemicals may increase in aquatic organisms of each successive trophic level due to increasing dietary exposures (e.g., increasing concentrations from algae, to zooplankton, to forage fish, to predatory fish) (EPA 2000a). In addition, because lipid content of aquatic organisms and the amount of organic carbon in the water column have been shown to affect bioaccumulation of nonionic organic chemicals, the national BAFs should be adjusted to reflect the lipid content of commonly consumed fish and shellfish and the freely dissolved fraction of the chemical in ambient water for these chemicals (EPA 2000a).

Even though the 2000 Methodology (EPA 2000a) and subsequent Technical Support documents (EPA 2003a, 2009) provide directions for the derivation of national BAF factors, EPA has, as yet, not calculated any BAFs for individual chemicals. Instead, when calculating national HHAWQC, EPA has replaced the factor "ΣFI_i*BAF_i" with the factor "FI*BCF," where BCF is the bioconcentration factor. A BCF is defined in the HHAWQC methodology document (2000a) as the ratio (in L/kg tissue) of the concentration of a substance in tissue of an aquatic organism to its concentration in the ambient water, in situations where the organism is exposed through the water only and the ratio does

not change substantially over time. Like the BAF, the BCF represents a ratio that relates the concentration of a chemical in water to its expected concentration in commonly consumed aquatic organisms, but unlike the BAF, it does not consider uptake from the diet or potential sources such as sediments. BAFs are intended to be reflective of real environmental exposures and thus also reflect factors such as bioavailability and biodegradation. Thus, BAFs can be higher or lower than BCFs.

The factor FI*BCF is a single calculation rather than the summing of multiple trophic levels. In the most recent National Recommended Water Quality Criteria: 2002, Human Health Criteria Calculation Matrix tables, the BCF values used are accompanied by a footnote that reads, "The fish tissue bioconcentration factor (BCF) from the 1980 criteria documents was retained unless otherwise noted" (EPA 2002b).

States are free to calculate their own site-specific BAFs or follow the current EPA practice of using BCFs.

5.6 Implicit Elements in the Derivation of HHAWQC

The derivation of HHAWQC incorporates assumptions about exposure that are not explicitly recognized in the formal equations shown in Table 3.1. These include bioavailability, cooking loss, exposure duration, and exposure concentration.

5.6.1 *Relative Bioavailability*

Bioavailability may be defined as the degree to which a substance contained in water, food, soil, air, or other media can be absorbed by living organisms. Bioavailability is an important component of toxicity assessment since absorption is an essential prerequisite to systemic toxicity and the degree of bioavailability is an important determinant of the ultimate exposure level. EPA's recommendations for the derivation of HHAWQC do not account for the bioavailability of substances and thus implicit is the assumption that the bioavailability of chemical substances in drinking water and fish tissue obtained from regulated waterbodies is the same as the bioavailability of those chemical substances in the studies from which the toxicity parameters (RfD, POD, cancer potency factor) were derived.

5.6.2 *Cooking Loss*

Chemical substances that may be present in fish tissue can be lost as part of the cooking process. Many substances that accumulate in fish tissues are associated with the lipid (i.e., fatty) content in the tissues. Most cooking practices result in partial loss of lipid and associated chemical substances. Other substances may be volatilized during the cooking process.

EPA's recommendations for the derivation of HHAWQC do not account for chemical loss during cooking. Thus implicit is the assumption that 100% of chemical substances present in raw fish remain in edible portions of fish tissue after cooking.

5.6.3 *Exposure Duration*

EPA's intentions for HHAWQC are to "minimize the risk of adverse effects occurring to humans from chronic (lifetime) exposures to substances through the ingestion of drinking water and consumption of fish obtained from surface waters" (EPA 2000a). Lifetime exposure is assumed to be 70 years. Thus the derivation of HHAWQC implicitly assumes that exposure to the criteria substance occurs continuously over 70 years.

5.6.4 *Exposure Concentration*

The combination of explicit toxicity and exposure elements as typically used in the HHAWQC derivation equation act to form an implicit assumption that the average concentration of regulated

substances in water and fish tissue exist in the environment at their maximum allowed concentrations at all times over the course of a person's lifetime (presumed to be 70 years).

6.0 PROTECTIVENESS, CONSERVATISM, AND THE COMBINED EFFECT OF CONSERVATIVE PARAMETER VALUE CHOICES IN DERIVATION OF HHAWQC

The Clean Water Act, from which authority for the designation of HHAWQC is derived, specifies, in a very broad sense, the level of protectiveness that should be embodied in the HHAWQC. The Clean Water Act includes language such as "protect the public health and welfare," "protect public health… from any reasonably anticipated adverse effects of each pollutant," and "[not] pose an unacceptable risk to human health."

In its HHAWQC methodology document, EPA provides another fairly broad description of its desired level of protectiveness: "Water quality criteria are derived to establish ambient concentrations of pollutants which, if not exceeded, will protect the general population from adverse health impacts from those pollutants due to consumption of aquatic organisms and water, including incidental water consumption related to recreational activities" (EPA 2000a). They also note that HHAWQC are usually derived to protect the majority of the general population from chronic adverse health effects and that they consider their target protection goal to be satisfied if the population as a whole will be adequately protected by the human health criteria when the criteria are met in ambient water (EPA 2000a).

In order to derive HHAWQC that are "adequately protective," EPA states that they have selected default parameter values that are "a combination of median values, mean values, and percentile estimates [that target] the high end of the general population" (EPA 2000a). EPA (2000a) "believes that this is reasonably conservative and appropriate to meet the goals of the CWA…"

The term "conservatism," in the context of derivation of HHAWQC, is used to describe the use of assumptions and defaults that are likely to overstate the true risks from exposure to substances in drinking water and fish tissues. The policy choice to use such overstatements is rooted in EPA's approach to dealing with uncertainty and variability in the data upon which defaults and assumptions are based.

Uncertainty is an inherent property of scientific data and thus of the process of risk assessment and the derivation of HHAWQC. Since uncertainty is due to lack of knowledge, it can be reduced by the collection of additional data, but never eliminated completely. Variability is an inherent characteristic of a population because people vary in their levels and types of exposures and their susceptibility to potentially harmful effects of the exposures (NRC 2009). Unlike uncertainty, variability cannot be reduced but can be better characterized with improved information (NRC 2009).

In a staff paper[3] on risk assessment principles and practices, EPA (2004) discussed its approach to dealing with uncertainty and variability:

> Since uncertainty and variability are present in risk assessments, EPA usually incorporates a "high-end" hazard and/or exposure level in order to ensure an adequate margin of safety for most of the potentially exposed, susceptible population, or ecosystem. EPA's high-end levels are around 90% and above…

[3] Staff paper prepared by the Risk Assessment Task Force through the Office of the Science Advisor at EPA. The document presents an analysis of EPA's general risk assessment practices.

> …EPA's policy is that risk assessments should not knowingly underestimate or grossly overestimate risks. This policy position prompts risk assessments to take a more "protective" stance given the underlying uncertainty with the risk estimates generated. Another framing policy position is that EPA will examine and report on the upper end of a range of risks or exposures when we are not very certain about where the particular risk lies… Further, when several parameters are assessed, upper-end values and/or central tendency values are generally combined to generate a risk estimate that falls within the higher end of the population risk range.
>
> [The] issue regarding the appropriate degree of "conservatism" in EPA's risk assessments has been a concern from the inception of the formal risk assessment process and has been a major part of the discussion and comments surrounding risk assessment…

Given the attention focused on the issue of "the appropriate degree of conservatism," it is not surprising that many researchers have studied ways in which uncertainty and variability can be better characterized and reduced, with the ultimate goal of developing risk estimates that better achieve EPA's stated goals of neither underestimating nor grossly overestimating risk without the use of highly conservative default assumptions. The sections below summarize some of these efforts and, where data are available, attempt to quantify the level of conservatism embodied in EPA's current policy choices related to the selection of parameters for use in calculating HHAWQC.

As means of examining the implications of conservatism embodied in the HHAWQC derivation process, several examples are presented in the following sections. The example substances, which include mercury, arsenic, methyl bromide, chlordane, bis (2-ethylhexyl)-phthalate (or BEHP), and polychlorinated biphenyls (PCBs), were chosen for illustration purposes because they represent broad chemical categories (e.g., metals and organics), current and legacy substances, and substances with low and high bioconcentration factors.

6.1 Toxicity Factors

Derivation of an RfD, selection of a POD and UFs, modeling the dose-response for carcinogens, and calculating the slope factor (m) are based on science, but also involve a variety of policy decisions. These policy decisions all embody some degree of conservatism. This section addresses in greater detail the conservatism associated with the lack of consideration of bioavailability and the selection of default values for uncertainty factors and cancer risk levels.

6.1.1 *Relative Bioavailability*

As noted in Section 5, an implicit assumption in the HHAWQC derivation equation is that the bioavailability of chemical substances in drinking water and fish tissue obtained from regulated waterbodies is the same as the bioavailability of those chemical substances in the studies from which the toxicity parameters (RfD, POD, cancer potency factor) were derived. However, a RfD is often based on an animal toxicity study in which exposures occurred via drinking water and for some substances, the bioavailability from fish tissue will be different from that from drinking water. In some cases, bioavailability from foods might be reduced by, for example, the formation of indigestible complexes with other food components or conversion to ionized forms that cannot pass through biological membranes and thus cannot be absorbed. For example, arsenic in drinking water is primarily inorganic arsenic, which is absorbed well, but almost all of the arsenic in fish tissues is organic arsenic, which is not highly bioavailable. Arsenic may also form insoluble complexes with, for example, iron, aluminum, and magnesium oxides, which limits bioavailability. For these substances, any particular dose consumed in fish tissue would result in a lower absorbed dose than the same dose consumed in drinking water. Thus, a RfD based on a drinking water study would be lower than a RfD based on a dose administered in fish tissue. Use of this lower RfD will overestimate the

potential hazards associated with the ingestion of fish tissue and will yield a lower HHAWQC (see, e.g., EPA 2000b).

EPA rarely provides information on the potential impacts of bioavailability on their RfDs and does not typically calculate alternative RfDs that might be used when expected exposures are via a route that is likely to result in reduced bioavailability. For example, most inorganic contaminants, particularly divalent cations, have bioavailability values of 20 percent or less from a food matrix, but are much more available (about 80 percent or higher) from drinking water (EPA 2000b). The Technical Support Document Volume 1: Risk Assessment (EPA 2000b) for the HHAWQC methodology document (EPA 2000a) does allow for the selection of an alternative RfD in cases where there is lower bioavailability of the contaminant when ingested in fish than when ingested in water and the existing RfD is based on a study in which the contaminant was administered through drinking water. However, in actual practice, this has not been done.

6.1.2 *Uncertainty Factors*

The UF methodology, which has its origins in the concept of "safety factors," has been the subject of discussion among scientists in many forums over the years. One of the most common issues of discussion is the scientific basis for the default factor of 10. It is generally accepted that selection of the first safety factors was based on qualitative judgment (Nair et al. 1995). Subsequently, however, attempts were made to justify the use of 10-fold factors based on data collected to characterize the uncertainty and variability associated with parameters such as intra- and interspecies differences.

One commonly accepted justification for the selection of 10 as the standard default uncertainty factor is that for any given chemical, the dose at which the endpoint of concern will be observed in the population of concern (e.g., the most sensitive subpopulation of humans) will be less than 10 times higher than the dose at which the endpoint of concern will be observed in the population that serves as a surrogate (e.g., average humans) for the purposes of deriving an RfD (Dourson et al. 1996).

The degree of conservatism embodied in the use of default factors of 10 has been examined by researchers who have summarized published data and determined the actual distributions of these ratios. Dourson et al. (1996) noted that "there is growing sentiment that …routine application [of 10-fold UFs] often results in overly conservative risk assessments."

For example, Nessel et al. (1995) were interested in the scientific basis for the application of an uncertainty factor of 10 when using a sub-chronic study instead of a chronic study to derive the RfD. The underlying assumption is that for any given chemical, the NOAELs and LOAELs of sub-chronic studies will be within a factor of 10 of the NOAELs and LOAELs of chronic studies. So, Nessel et al. (1995) compared NOAELs and LOAELs from 23 different sub-chronic oral toxicity studies to the NOAELs and LOAELs of chronic studies that were identical except for the study duration. The mean and median $NOAEL_{subchronic}/NOAEL_{chronic}$ ratios were 2.4 and 2.0, respectively. Twenty-two of the 23 studies had NOAEL ratios of 5 or less; only one had a ratio of 10. The LOAEL ratios' mean and median were also 2.4 and 2.0, with all 23 studies having $LOAEL_{subchronic}/LOAEL_{chronic}$ ratio of 5 or less. So, based on this study, an uncertainty factor of 5 is sufficient to account for differences between sub-chronic and chronic studies in 98% of studies. Kadry et al. (1995) reported similar findings as did the review conducted by Dourson et al. (1996).

Similarly, differences between LOAELs and NOAELs are typically less than 10 fold. Ninety-six percent of all LOAEL-to-NOAEL ratios in one study were 5 or less and 91% were 6 or less in another (summarized by Dourson et al. 1996). Kadry et al. (1995) reported similar findings.

The decision to use conservative default UFs has particular significance on the overall conservatism of the RfD that is derived using the UFs. Gaylor and Kodell (2000) examined this issue and quantified the increasing degree of conservatism as the number of default UFs applied increases.

When ratios are calculated for UFs as described in the two previous paragraphs, the distributions of these ratios are lognormal, with the value of 10 typically representing the 95th percentile (Swartout et al. 1998). Gaylor and Kodel (2000) calculated the uncertainty factors that would be required to maintain an overall 95th percentile level when multiple default uncertainty factors are applied. They found that for the use of any two UFs, for which the current default total UF would be 100, the UF required to maintain the 95th percentile level ranged from 46 to 85. For the use of any three UFs, for which the current default total UF would be 1000, the UF required to maintain the 95th percentile level ranged from 190 to 340. Swartout et al. (1998) conducted a similar analysis using a different technique and reported similar findings, concluding that default UFs of 100, 1000, and 3000, for application of two, three, and four UFs, respectively, can be replaced with UFs of 51, 234, and 1040, while maintaining the 95th percentile level.

If a composite UF calculated to maintain the desired 95th percentile level is used instead of the default values of 100, 1000, and 3000, the resultant RfD and subsequently calculated HHAWQC could be as much as 5x higher. For example, if the RfD for methyl bromide was calculated using an UF of 340 (the top of the range calculated by Gaylor and Kodel (2000)) instead of 1000, the RfD would be 0.0041 mg/kg/day rather than the existing value of 0.0014 mg/kg/day. This would yield a HHAWQC of 139 µg/L rather than 47 µg/L.

6.1.3 *Cancer Risk Levels*

EPA chose to use the one-in-one-million (10^{-6}) risk level as the default value when calculating HHAWQC because it believes this risk level "reflects an appropriate risk for the general population" (EPA 2000a). However, EPA (2000a) also notes that risk levels of 10^{-5} for the general population and 10^{-4} for highly exposed populations are acceptable.

The frequent use of the 10^{-6} risk level to represent "an appropriate risk for the general population" appears to be simply a policy choice with no solid scientific basis. In a paper[4] presented at the 84th Annual Meeting of the Air & Waste Management Association in 1991, Kelly reported that:

> …despite its widespread use: no agencies we contacted could provide documentation on the origins of 10^{-6}; its origin was determined to be a completely arbitrary figure adopted by the FDA as an "essentially zero" level of risk for residues of animal drugs; there was virtually no public debate on the appropriateness of this level despite requests by the FDA; this legislation stated that 10^{-6} was specifically not intended to be used as a definition of acceptable risk; 10^{-6} is almost exclusively applied to contaminants perceived to be of great risk (hazardous waste sites, pesticides); and 10^{-6} as a single criterion of "acceptable risk" is not and has never been in any EPA legislation or guidance documents.

The decision of which cancer risk level to use in any particular circumstance is, for the most part, something that has evolved over many years through policy positions put forth in various EPA reports and legislation, but the idea that cancer risk levels between 10^{-6} and 10^{-4} are acceptable have become widely accepted among the different EPA programs. For example, the 1990 Clean Air Act Amendments endorse a 1989 EPA assessment for benzene in which EPA identified 1 in 10 thousand (10^{-4}) as being an "acceptable" risk level and 1 in a million (10^{-6}) as representing "an ample margin of safety." An EPA Region 8 superfund site discussion[5] stated that:

> In general, the USEPA considers excess cancer risks that are below about 1 chance in 1,000,000 (1×10^{-6} or 1E-06) to be so small as to be negligible, and risks above 1E-04 to be

[4] Available online at http://www.deltatoxicology.com/pdf/10-6.pdf
[5] http://www.epa.gov/region8/r8risk/hh_risk.html

> sufficiently large that some sort of remediation is desirable. Excess cancer risks that range between 1E-06 and 1E-04 are generally considered to be acceptable, although this is evaluated on a case-by-case basis and EPA may determine that risks lower than 1E-04 are not sufficiently protective and warrant remedial action.

Jones-Otazo et al. (2005) compared screening level risk assessment practices among different regulatory agencies and found that most have adopted acceptable risk levels in the same range as EPA. The European Union (EU) and World Health Organization (WHO) both identify risks in the range of 10^{-6} to 10^{-4} as acceptable, while Health Canada uses 10^{-5} as their acceptable risk level (Jones-Otazo et al. 2005). With respect to cancer risks associated with pollutants in drinking water, WHO uses a 10^{-5} risk level: "In this and previous editions of the Guidelines [for Drinking Water Quality], an upper-bound excess lifetime risk of cancer of 10^{-5} has been used, while accepting that this is a conservative position and almost certainly overestimates the true risk" (WHO 2008).

Population Risk - One factor that has a significant effect on the magnitude of acceptable risk is the size of the affected population. Exposure of a population of 1 million to a carcinogen at the risk level of 1 in a million theoretically results in one additional case of cancer among those 1 million people over the course of 70 years. If the size of the population of concern is decreased to 100,000 instead of 1 million, the theoretical additional cases of cancer among those 100,000 individuals decreases to only 0.1 case over the course of 70 years. Population risk is an important consideration in selecting a fish intake rate for use in developing AWQC because as the size of the exposed population decreases, the population risks also decrease when the same target risk level is used. The higher the FI rate selected for a particular population, the smaller the population to which that rate applies. For example, if the FI rate selected is a 95th percentile rate, it is assumed that it is protective of all but 5 percent of the exposed population or 50,000 of the 1 million people provided in the example above. Thus, if the same target risk level of 1E-06 is used with this reduced population, the resulting population risk is 0.05 excess cancers within a population of 1 million people. In other words, in order to reach the target risk of 1 excess cancer, it would be necessary for a population of 20 million people to have lifetime exposures equivalent to the estimated exposure conditions. This topic is discussed in much greater detail in Appendix A, Section 4.0 Population Risk.

This concept is particularly relevant to HHAWQC derivation because very small populations of fish consumers with high intake rates are frequently identified as being of special concern during the HHAWQC derivation process. The HHAWQC methodology document states that a risk level of 10^{-4} for highly exposed populations is acceptable (EPA 2000a). This is sometimes interpreted as meaning that highly exposed populations are not as well protected by the HHAWQC. However, as noted by Kocher (1996) in a discussion of cancer risks at hazardous waste sites, "if only a small population would be at greatest risk, the expected number of excess cancers corresponding to individual risks at the *de minimis* level of 10^{-4} would still be [essentially] zero." Travis et al. (1987) reviewed 132 federal regulatory decisions and concluded that in actual practice, for small population risks, the *de minimis* lifetime risk was considered to be 10^{-4}.

Given that the 10^{-4} risk level has been identified as an acceptable/*de minimis* risk level for highly exposed populations, it may be useful to consider exactly what that risk level represents in terms of FI. If the default FI of 17.5 g/day represents a 10^{-6} target risk level, then a highly exposed population that eats as much as 1750 g/day will still be protected at a 10^{-4} risk level.

6.2 Explicit and Implicit Exposure Factors

The specific exposure factors that EPA uses in the derivation of HHAWQC include human body weight, drinking water consumption rates, and fish ingestion rates. In the HHAWQC methodology document, EPA states that the selection of specific exposure factors is "based on both science policy decisions that consider the best available data, as well as risk management judgments regarding the

overall protection afforded by the choice in the derivation of AWQC" (EPA 2000a). This section addresses the levels of conservatism represented by the default values selected by EPA for individual explicit and implicit exposure factors.

6.2.1 *RSC*

The RSC determines what portion of the RfD will be allocated to the consumption of water and fish from regulated waterbodies. For example, if the RfD for a particular substance is 1 mg/kg/day and the RSC is 20%, then the HHAWQC must be set such that exposures to that substance via water and fish can be no more than 0.2 mg/kg/day. Thus, the lower the RSC, the lower the HHAWQC that will be derived.

Although EPA (2000a) does provide a decision tree methodology for calculating chemical- or site-specific RSCs, the lowest allowable value, 20%, is specified as the default RSC by EPA in its calculations of HHAWQC. EPA explains this in the HHAWQC methodology document (EPA 2000a) with the statement that "[the default value of 20%] is likely to be used infrequently with the Exposure Decision Tree approach, given that the information [required to calculate a chemical-specific RSC]…should be available in most cases. However, EPA intends to use 20 percent…" This statement clearly indicates that for most chemicals, an RSC greater than 20% is appropriate, but EPA has chosen to use the most conservative 20% default value. Use of an RSC of 20% when data indicate that a larger percentage is more appropriate can result in as much as a 4-fold reduction in the HHAWQC.

The California Office of Environmental Health Hazard Assessment (OEHHA) concluded that the default use of an RSC of 20% is "unreasonably conservative for most chemicals" (Howd et al. 2004). For 22 of the 57 chemicals listed by Howd et al. (2004), a RSC value greater than 20% was used in the calculation of California Public Health Goals for those chemicals in drinking water. Howd et al. (2004) also noted that "[a] default RSC of 0.2 is based on tradition, not data."

A recent Government Accountability Office report (GAO (2011) calculated the effect of using different RSC factors on the determination of drinking water health reference levels (HRLs) for a hypothetical chemical with an RfD of 0.5 µg/kg/day. While holding all other variables constant, RSC values of 20%, 50%, and 80% were inserted into the equation. The corresponding HRLs were 3.5 ppb (20%), 8.8 ppb (50%), and 14 ppb (80%).

A RSC may be calculated in two ways. The subtraction method allocates 100% of the RfD among the various sources of exposure. So, the daily exposure from all exposure routes other than drinking water and fish consumption are first subtracted from the RfD, then the remainder of the RfD is allocated to drinking water and fish consumption. The percentage method does not attempt to quantify exposures from other sources, but rather simply allocates a percentage of total exposure to drinking water plus fish consumption and to other sources.

EPA has chosen to use the percentage method as the default approach. EPA states that in most cases, they lack adequate data to use the subtraction method and that the percentage method is more appropriate for situations in which multiple media criteria exist (EPA 2000a). The GAO report (GAO 2011) notes that the percentage method is considered to be the more conservative option and generally yields a lower water quality criteria value. The GAO illustrated the difference in outcome by using the data for a hypothetical chemical to calculate drinking water health reference values (HRV) using both methods. Using the subtraction method, the HRV was 12.3 ppb. Using the percentage method, the HRV was 8.8 ppb, a 1.4-fold reduction.

6.2.2 *Body Weight*

The HHAWQC methodology document (EPA 2000a) recommends using a BW of 70 kg. This number was chosen in part because it is in the range of average values for adults reported in several studies and in part because it is the default body weight used in IRIS calculations. However, in 2011, EPA released an updated edition of the Exposure Factors Handbook (EPA 2011b). Based on data from the National Health and Nutrition Examination Survey (NHANES) 1999-2006, the new handbook recommends a mean BW value of 80 kg for adults.

The RfD is defined as "an estimate (with uncertainty spanning approximately an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious effects over a lifetime" (EPA 2000b). The RfD expresses this daily exposure as a function of body weight (mg of chemical per kg of body weight), so the daily exposure that is likely to be without appreciable risk will be lower for an individual with a lower body weight than for an individual with a higher body weight. Thus, the lower the body weight used in the calculation of the HHAWQC, the lower the resulting criteria. For this reason, the choice to use 70 kg as the default body weight adds to the conservatism of the HHAWQC and yields criteria values approximately 12.5% lower than those calculated using the more accurate population mean of about 80 kg BW recommended by EPA in the latest Exposure Factors Handbook (EPA 2011b).

6.2.3 *Drinking Water Intake*

EPA (2000a) cites several reasons for including the drinking water exposure pathway in the derivation of HHAWQC:

(1) Drinking water is a designated use for surface waters under the CWA and, therefore, criteria are needed to assure that this designated use can be protected and maintained.

(2) Although rare, there are some public water supplies that provide drinking water from surface water sources without treatment.

(3) Even among the majority of water supplies that do treat surface waters, existing treatments may not necessarily be effective for reducing levels of particular contaminants.

(4) In consideration of the Agency's goals of pollution prevention, ambient waters should not be contaminated to a level where the burden of achieving health objectives is shifted away from those responsible for pollutant discharges and placed on downstream users to bear the costs of upgraded or supplemental water treatment.

These reasons make it clear that 2 L/day was selected as the default water consumption rate in support of larger goals related to pollution prevention and maintenance of designated use and does not represent a consideration of actual direct risk of adverse effect to any individual consumer. As EPA itself noted, it would be rare for anyone to use untreated surface water as a source of drinking water. The only direct consumption of untreated surface waters that might be considered to be routine is incidental ingestion during swimming, for which the EPA (2011b) recommended upper percentile default rates are 120 mL/hr for children and 71 mL/hour for adults. Using the 95^{th} percentile estimate for time spent swimming each month (181 minutes) (EPA 2011b), annual daily average water consumption rates of 0.012 L/day (children) and 0.007 L/day (adults) can be calculated.

The default water consumption rate of 2L/day represents reported consumption of water from "community water," which is defined as tap water from a community or municipal water source. It does not represent a realistic level of consumption of untreated surface waters, which is likely to occur only as an incidental event of water-related recreational activities. However, by using 2 L/day in the calculation of the HHAWQC, EPA is deriving criteria values that are based on the assumption

that the general population is indeed consuming 2 L/day of untreated surface water. Thus, the use of 2 L/day in the HHAWQC can insert a significant level of conservatism into the calculations.

The impact of the use of 2 L/day varies according to the BAF/BCF of the chemical. For chemicals with high BAFs/BCFs, the impact of drinking water intake on the ultimate HHAWQC is minimal due to the much larger contribution of the "fish intake x BAF" factor in the equation. However, for substances with low BAFs/BCFs, the impact is much greater. Table 6.1 shows the effect of changing drinking water intake rates on the HHAWQC of some example compounds with different BCFs.

Table 6.1 Human Health Ambient Water Quality Criteria Calculated for Varying Drinking Water Intakes

		HHAWQC (µg/L)		
Compound	BCF	DI = 2L/day (current default)	DI = 1L/day (mean DI for adults[1])	DI = 0.007L/day (ingestion while swimming)
Methyl bromide	3.75	47.4	91.96	1,349.40
Arsenic	44	0.017	0.031	0.137
BEHP[2]	130	1.17	1.53	2.19
Chlordane	14100	0.000804	0.000807	0.000811
PCBs	31200	0.0000639	0.0000640	0.0000641

[1]EPA 2011
[2]Bis(2-ethylhexyl)-phthalate

6.2.4 *Fish Consumption*

Note: Appendix A of this document contains a thorough treatment of topics related to the collection and interpretation of data used for deriving fish intake rates (FIs) (or fish consumption rates, FCRs) and applied in the derivation of HHAWQC. The appendix was prepared by Ellen Ebert, a recognized expert on interpretation of fish collection and consumption survey data.

Surveys of Fish Consumption - FIs tend to be overestimated in most surveys for a number of reasons. Individuals who respond to surveys with long recall periods tend to overestimate their participation in activities that are pleasurable to them. Creel surveys tend to be biased toward higher representation of more avid anglers who have high success rates and, thus, may consume at higher rates than the typical angler population. Short-term diet recall surveys tend to incorrectly classify people who eat a particular type of food infrequently as "non-consumers" and overestimate consumption by "consumers." Often people classified as "non-consumers" are excluded from the summary statistics of short-term diet recall survey resulting in an overestimate for ingestion rates for the entire survey population. Finally, when specific information is lacking from survey data, decisions are generally made during analysis of the survey data to ensure that consumption will not be underestimated (e.g., relatively large meal sizes will be substituted for unknown meal sizes, frequency of meals reported will be assumed to be consistent throughout the year regardless of fishing season, etc.) More detailed discussion of surveys used to determine FIs may be found in Appendix A.

Consumption of Marine and Imported Fish - As noted in Section 5.4 above, EPA's HHAWQC methodology document recommends that fish consumption rates be based on consumption of

freshwater and estuarine species only and that any consumption of marine species of fish should be accounted for in the calculation of the RSC (EPA 2000a). However, the surveys used as the basis for EPA's recommended default fish consumptions rates collected information on the total consumption of fish of any species and from all sources, e.g., purchased or sport-caught fresh, frozen, or canned fish from local, domestic, or international sources (EPA 2011b). Surveys that collect information on the specific species consumed reveal that the majority of finfish consumed by Americans are marine species (Table 6.2). Also, as reported by the NOAA Fisheries Service[6], most of the seafood consumed in the U.S. is not caught in U.S. waters. In fact, about 86 percent of the seafood consumed in the U.S. is imported. Thus, the fish consumption rate used in the calculation of HHWQC significantly overestimates consumption of fish from regulated freshwater/estuarine waters by the majority of the population.

Table 6.2 Per Capita Consumption of Seafood in the U.S. – Top 10 Species (MBA 2011)

Type of Seafood	Pounds Consumed per Person/Year	Additional Comments
Shrimp	4	85% imported, mostly farmed, some wild caught
Canned tuna	2.7	Marine species
Salmon	2	Marine species
Tilapia	1.5	Farmed fish, most are imported
Pollack	1.2	Marine species
Catfish	0.8	Farmed fish, from both domestic and imported sources
Crab	0.6	
Cod	0.5	Marine species
Pangasius	0.4	Primary source is fish farms in Asia
Clams	0.3	

Additional discussion of the basis for excluding marine fish from fish consumption rate determinations may be found in Appendix B, which addresses issues relevant to the accumulation of persistent, bioaccumulative, and toxic chemicals by salmon in the context of the development of fish consumption rates in the state of Washington.

Consumption of Fish from Regulated Waters - Default assumptions that the general population consumes fish taken from contaminated water bodies every day and year of their entire life represent additional conservative assumptions. When applied to establishing permit limits or the risk

[6] http://www.noaanews.noaa.gov/stories2011/20110907_usfisheriesreport.html

assessment of a specific site or waterbody, the HHAWQC inherently assumes that 100 percent of the fish consumed over a lifetime are taken from that waterbody. This may be a reasonable assumption when the chemical constituents of concern are ubiquitous so that it is possible that individuals might receive similar levels of exposure even if they fish multiple waterbodies, but is likely to overestimate potential risk when applied to a single waterbody or one that is unique in terms of its chemical concentration or sources of the chemical in question. While it is possible individuals could obtain 100 percent of their fish from a single waterbody, this is not typical unless the waterbody is very large or represents a highly desirable fishery. In addition, individuals are likely to move many times during their lifetimes and, as a result of those moves, may change their fishing locations and the sources of the fish they consume. Finally, it is likely that most anglers will not fish every year of their lives. Health issues and other demands, like work and family obligations, will likely result in no fishing activities or reduced fishing activities during certain periods of time that they live in a given area. Thus, these assumptions add conservatism to the derivation of HHAWQC.

Implied Harvest Rate - EPA's default rate of 17.5 g/day indicates the amount of fish that is actually consumed. In order to achieve that rate, one must harvest 58 g/day of whole fish [assuming EPA's recommended edible portion of 30 percent (EPA 1989)] to yield 17.5 g/day of edible fish. When annualized, this results in 21,300 grams of fish per person or 47 pounds of fish per consumer per year. When considered over the 70-year exposure period (as assumed in the HHAWQC calculation), this results in the total removal of 3,300 pounds of fish/person during that period. In addition, if that individual is providing fish to a family of four, it would be necessary to remove roughly 13,000 pounds of fish from a single waterbody during that 70-year span. This represents a significant level of fishing effort and harvest and likely represents a substantial overestimate of any actual fish that is likely to be harvested from a single waterbody by a single individual.

Source of HHAWQC Default FIs - The food intake survey upon which the default fish consumption rates were based were short-term surveys. Numerous researchers have reported that the long-term average daily intake of a food cannot be determined using these short-term cross-sectional surveys (Tran et al. 2004). The use of short-term surveys has been shown to overestimate long-term food intakes in the upper percentile ranges (Tran et al. 2004) that are typically used by EPA in exposure assessments, especially for infrequently consumed foods (Lambe and Kearney 1999) like fish. Additional discussion of the limitations of the use of short-term survey data on fish consumption may be found in Appendix A, Section 3.2.2.

Summary - The fish consumption rates used in calculating HHAWQC can have a significant impact on the resulting HHAWQC. This is because the HHAWQC are proportional to the fish consumption rates (as the rate increases, the HHAWQC decreases) and there is substantial variability in the rates of fish consumption among the consuming population. In addition, the potential exposure through the fish consumption pathway is dependent upon a number of different variables including the types of fish consumed, the sources of those fish, and the rates at which they are consumed. The quantification of fish consumption rates is complicated by the methods used to collect consumption information, the availability of fish from regulated sources, and the habits of the targeted population of fish consumers.

The selection of fish consumption rates when calculating HHAWQC is discussed in more detail in Appendix A.

6.2.5 *Cooking Loss*

The derivation of HHAWQC is based on the assumption that there will be no loss of chemicals from fish tissues during the cooking process. However, numerous studies have shown that cooking reduces the levels of some chemicals. For example, Zabik et al. (1995) reported that cooking significantly reduced levels of the DDT complex, dieldrin, hexachlorobenzene, the chlordane complex, toxaphene,

heptachlor epoxide, and total PCBs. Similarly, Sherer and Price (1993), in a review of published studies, reported that cooking processes such as baking, broiling, microwaving, poaching, and roasting removed 20-30% of the PCBs while frying removed more than 50%.

In its development of Fish Contaminant Goals (FCGs) and Advisory Tissue Levels, the State of California uses a cooking reduction factor to account for cooking loses for some chemicals:

> FCGs take into account organochlorine contaminant loss during the cooking process. The concentration of PCBs and other organic contaminants in fish are generally reduced by at least 30 percent, depending on cooking method… As such, a cooking reduction factor of 0.7 was included in the FCG equation for organic compounds (allowing for 70 percent of the contaminant to remain after cooking) (CA 2008).

By not incorporating a chemical-specific factor to adjust for cooking loss, the exposure level from fish consumption will be overestimated for organic compounds, thus lending an additional layer of conservatism to the resulting HHAWQC.

6.2.6 *Exposure Duration*

As noted in Section 5, exposure duration is an implicit element in the derivation of HHAWQC and a value of 70 years, or an approximate lifetime, is assumed. While average lifetimes may be approximated by 70 years, it is generally considered conservative to assume that an individual would be continuously exposed to substances managed through the development of HHAQWC because waters contaminated with such substances do not exist everywhere and it is unlikely that many persons would reside only in contaminated areas, and drink and fish only in these waters for an entire lifetime. Choosing to assume a 70-year exposure duration may be justified in cases where a pollutant is ubiquitous in the environment and thus it could reasonably be assumed that ingestion of drinking water and locally caught fish from essentially all freshwater locations would lead to similar levels of exposure. There is little evidence, however, supporting the ubiquity of most substances for which HHAWQC have been established (though an exception might be justified for mercury or other pollutants for which atmospheric deposition is the dominant mechanism contributing substances to surface waters).

Perhaps more significantly, however, it is uncommon for people to reside in a single location for their entire life. EPA's Exposure Factors Handbook (EPA 2011) contains activity factors, including data for residence time, from several US studies. Table 6.3 summarizes some of these results.

Table 6.3 Values for Population Mobility

	Mean	90th Percentile	95th Percentile
Residential Occupancy Period (Johnson and Capel 1992)	12 years	26 years	33 years
Current Residence Time (US Census Bureau 2008)	8 years (median) 13 years (mean)	32 years	46 years

As with other survey results, there is some uncertainty and potentially some bias associated with the residency periods reported in these studies. Additional studies are discussed (EPA 2011) concerning the distance people move, when they do move. However, the data clearly suggest that the central tendency (mean or median) and upper percentile values are substantially less than the 70 year

exposure period assumed by EPA. The assumption of a 70 exposure duration overestimates median exposure duration by 8-fold, mean exposure duration by approximately 6-fold and the 90th percentile by 2- to 3-fold. Thus, the choice to use 70 years is conservative for most non-ubiquitous chemicals. Table 6.4 shows the effect on some example HHAWQC when assuming exposure durations of 70 and 30 years.

Table 6.4 HHAWQC Calculated Based on 70 and 30 Year Exposure Durations

	HHAWQC (µg/L)	
Compound	70 year exposure duration	30 year exposure duration
Arsenic	0.017	0.040
BEHP	1.17	2.73
Chlordane	0.000804	0.00187
PCBs	0.0000639	0.000149

6.2.7 *Exposure Concentration*

As noted in Section 5, implicit with the derivation of HHAQWC is the assumption that both the water column and fish tissue concentrations exist at their maximum allowed values for the entire 70 year exposure duration. In reality, water column concentrations vary over time and space. The assumption that concentrations are always the maximum allowed is unnecessarily conservative as a practical matter because, as described in the following paragraphs, regulations governing water quality in the US would not allow a substance to persist in a water body at the HHAQWC concentration for such a period.

EPA's Impaired Waters and Total Maximum Daily Load Program provides guidance to states concerning when waters are considered to be impaired. The EPA guidance is not specific as to recommendations for identifying stream impairments due to exceedances of HHAWQC and many state impaired stream listing methodologies lack specific provisions unique to the basis for establishing HHAWQC (i.e., exposure over a 70 year lifetime). However, it is common that states will consider listing a stream that exceeds WQC for chronic aquatic life (i.e., the CCC) and human health more than 10% of the time (i.e., the "10% rule"). Indeed, EPA guidance for listing impaired surface waters (EPA 2003b) states:

> "Use of the '10% rule' in interpreting water quality data in comparison with chronic WQC will generally be more appropriate than its use when making attainment determinations where the relevant WQC is expressed "concentration never to exceed ___, at any time." Chronic WQC are always expressed as average concentrations over at least several days. (EPA's chronic WQC for toxics in freshwater environments are expressed as 4-day averages. On the other extreme, EPA's human health WQC for carcinogens are calculated based on a 70-year lifetime exposure period.) Using the '10% rule' to interpret data for comparison with chronic WQC will often be consistent with such WQC because it is unlikely to lead to the conclusion that water conditions are better than WQC when in fact, they are not."

The guidance above suggests that listing of waters using the 10% rule is likely to be over protective for chronic aquatic life criteria. That is, it is considered unlikely that a water exceeding the chronic WQC 10% or less of the time would exist, on average, at the criterion value for the 4-day averaging period on which chronic WQC are based. By this same logic, it is an essentially impossible scenario

that a water exceeding a HHAWQC 10% or less of the time would average at the criterion value for the 70 year averaging period on which HHAWQC are based.

It may be more realistic, instead, to predict a mean or median water column concentration using the HHAWQC as an upper percentile value occurring in the stream. Considering the 10% rule, one might predict the average water column concentration by assuming that the HHAWQC is the 90th percentile value in a distribution of water column concentrations existing over 70 years. By way of example, Table 6.5 illustrates the effect of variable stream concentrations on the ratio of the 90th percentile concentration to the mean concentration. An approximately normal distribution is assumed for these examples.

Table 6.5 Ratio of 90th Percentile Upper Bound Concentration to the Mean (normal distribution)

	Assumed Distribution	HHAWQC	Standard Deviation and Coefficient of Variation[1]	Estimated Mean[2]	Ratio HHAWQC/Mean
Substance X	Normal	1	0.25	0.68	1.5x
Substance Y	Normal	1	0.50	0.36	2.8x
Substance Z	Normal	1	0.60	0.23	4.3x

[1]The coefficient of variation (or relative standard deviation) is the ratio of the standard deviation to the mean and represents the degree of relative variability of the data around the mean.
[2]The 90th upper percentile of a normal distribution lies about 1.28 standard deviations from the mean.

The same general characteristic would be expected for stream concentrations that are log-normally distributed, which is a more common situation. Assuming that the values used in the normal distribution case in the previous table apply to the logarithms of the original data, a ratio of the antilogs of the HHAWQC (90th percentile value) and mean values in the normal distribution case can be calculated. Results are shown below in Table 6.6.

Table 6.6 Ratio of 90th Percentile Upper Bound Concentration to the Mean (lognormal distribution)

	Assumed Distribution	Antilog of HHAWQC	Standard Deviation of log concentrations	Estimated Geometric Mean[1]	Ratio HHAWQC/Geometric Mean
Subst. X	Lognormal	10	0.25	4.8	2.1x
Subst. Y	Lognormal	10	0.50	2.3	4.4x
Subst. Z	Lognormal	10	0.60	1.7	5.9x

[1]The geometric mean is equal to the antilog of the Estimated Mean in the normal distribution table.

As can be seen in Tables 6.5 and 6.6, the actual mean can be a small fraction of the upper 90th percentile value. In these examples the degree of conservatism embodied in the HHAWQC value ranges between 1.5x and 5.9x.

6.3 Compounded Conservatism

Compounded conservatism is the term used to describe the "impact of using conservative, upper-bound estimates of the values of multiple input variables in order to obtain a conservative estimate of risk…" (Bogen 1994). Bogen (1994) pointed out that "safety or conservatism initially assumed for each risk component may typically magnify, potentially quite dramatically, the resultant safety level of a corresponding final risk prediction based on upper-bound inputs." In the HHAWQC derivation process, compounded conservatism plays a role both in the determination of individual factors of the Equations 3.1, 3.2, and 3.3 (i.e., in the toxicity factors and explicit and implicit exposure elements) and in the equations' use of multiple factors, each based on upper bound limits and/or conservative assumptions.

In addition to the conservatism embodied in the selection of individual components of the calculations (both explicit and implicit), the fundamental underlying assumption, which is that the most sensitive subpopulations will be exposed to maximum allowable concentrations over a full lifetime, is a highly unlikely and highly protective scenario. For example, the derivation of HHAWQC is based on the assumptions that an individual will live in the same place for their entire life (70 years) and that 100% of the drinking water and fish consumed during those 70 years will come from the local water body being regulated.

The suggestion that the use of multiple default factors based on upper bound limits and/or conservative assumptions lead to a situation of compounded conservatism has been the subject of considerable discussion (see Section 6.0). However, in a staff paper, EPA suggests that "when exposure data or probabilistic simulations are not available, an exposure estimate that lies between the 90th percentile and the maximum exposure in the exposed population [should] be constructed by using maximum or near-maximum values for one or more of the most sensitive variables, leaving others at their mean values" (EPA 2004). This appears to be an acknowledgement that adequately protective assessments do not require that each, or even most, component parameter(s) be represented by a 90th or 95th percentile value.

Similarly, in the 2005 Cancer Risk Assessment Guidelines, EPA (2005) stated:

> Overly conservative assumptions, when combined, can lead to unrealistic estimates of risk. This means that when constructing estimates from a series of factors (e.g., emissions, exposure, and unit risk estimates) not all factors should be set to values that maximize exposure, dose, or effect, since this will almost always lead to an estimate that is above the 99th-percentile confidence level and may be of limited use to decision makers.

Viscusi et al. (1997) provided a simple example to illustrate compounded conservatism. In Superfund exposure assessments, EPA states that they consider "reasonable worst case" exposures to be in the 90-95th percentile range (Viscusi et al. 1997). However, the use of just three conservative default variables (i.e. 95th percentile values) yields a reasonable worst case exposure in the 99.78th percentile. Adding a fourth default variable increases the estimate to the 99.95th percentile value. In a survey of 141 Superfund sites, the authors reported that the use of conservative risk assessment parameters in site assessments yields estimated risks that are 27 times greater than those estimated using mean values for contaminant concentrations, exposure durations, and ingestion rates.

In a recent report on the economics of health risk assessment, Lichtenberg (2010) noted that the use of conservative default parameters is intended to deliberately introduce an upward bias into estimates of risk. Lichtenberg (2010) also stated that "the numbers generated by such procedures can't really be

thought of as estimates of risk, since they bear only a tenuous relationship to the probability that individuals will experience adverse health consequences or to the expected prevalence of adverse health consequences in the population." Indeed, he pointed out that the number of actual cancer deaths that can be attributed to all environmental and occupational causes is much lower than the number that is predicted by risk assessments (Doll and Peto 1981, as cited by Lichtenberg 2010). Lichtenberg (2010) describes concerns about compounded conservatism by saying:

> …regulators continue to patch together risk estimates using a mix of "conservative" estimates and default values of key parameters in the risk generation process. Such approaches give rise to the phenomenon of compounded conservatism: The resulting estimates correspond to the upper bound of a confidence interval whose probability is far, far greater than the probabilities of each of the components used to construct it and which depends on arbitrary factors like the number of parameters included in the risk assessment.

6.4 Summary

Most of the components of the equations used to calculate HHAWQC contain some level of conservatism. The toxicity factors in and of themselves contain multiple conservative parameters, leading to a compounding of conservatism in their derivation. The default RSC is the most conservative allowable level derived using the more conservative of two possible approaches. The default body weight of 70 kg is 10 kg less than the EPA currently recommended value of 80 kg. The derivation process for the HHAWQC does not take into account expected cooking losses of organic chemicals. The compounded conservatism that results from the use of multiple conservative factors yields a HHAWQC that provides a margin of safety that is considerably larger than EPA suggests is required to be protective of the population, even when sensitive or highly exposed individuals are considered. Tables 6.7 and 6.8 illustrate the impact of replacing just two default parameters, body weight and drinking water intake, with average values and allowing for cooking loss on the HHAWQC for methyl bromide and bis(2-ethylhexyl)-phthalate (BEHP).

Table 6.7 Impact of Multiple Conservative Defaults/Assumption on Methyl Bromide HHAWQC

Parameters Used	HHAWQC (µg/L)
Default	47
Factor of 0.7 included for cooking loss	48
Factor of 0.7 included for cooking loss + DI default (2 L/day) replaced by mean value of 1 L/day	94
Factor of 0.7 included for cooking loss + DI default (2 L/day) replaced by mean value of 1 L/day + Default BW of 70 kg replaced by current EPA recommended BW of 80 kg	107

Table 6.8 Impact of Multiple Conservative Defaults/Assumption on BEHP HHAWQC

Parameters Used	HHAWQC (µg/L)
Default	1.17
Factor of 0.7 included for cooking loss	1.39
Factor of 0.7 included for cooking loss + DI default (2 L/day) replaced by mean value of 1 L/day	1.93
Factor of 0.7 included for cooking loss + DI default (2 L/day) replaced by mean value of 1 L/day + Default BW of 70 kg replaced by current EPA recommended BW of 80 kg	2.20

Not only do the individual components of the equations represent a variety of conservative assumptions, the underlying premise upon which calculations of HHAWQC are based is itself highly conservative. It assumes that 100 percent of the fish and drinking water consumed by an individual over a 70 year period is obtained from a single waterbody (or that a chemical is ubiquitous in all water), that the chemical is present at the HHAWQC at all times, an individual consumes fish every year at the selected upper bound consumption rate, and that no loss of the chemical of interest occurs during cooking.

In addition, the toxicological criteria used to develop the HHAWQC have been selected to be protective of the most sensitive individuals within the exposed population and have been combined with conservative target risks. It is unlikely that this combination of assumptions is representative of the exposures and risks experienced by many, if any, individuals within the exposed population.

Tables 6.9 and 6.10 summarize the primary sources of conservatism found in both the explicit and implicit toxicity and exposure parameters of HHAWQC derivation and, for some parameters, quantify the extent of that conservatism.

Table 6.9 Conservatism in Explicit Toxicity and Exposure Parameters

Explicit Exposure Parameter	Default Value	Represents:	Default is conservative because:	Impact of conservatism on HHAWQC (if known)
RfD	N/A	Estimate of daily exposure likely to be without appreciable risk of adverse effects over a lifetime	Bioavailability not typically considered, effects of compounded conservatism in use of multiple UFs	Larger RfD yields higher HHAWQC, magnitude uncertain and varies between compounds
RSD	N/A	Dose associated with incremental risk level of 10^{-6}	based on upper bound risk estimate	Magnitude uncertain, varies between compounds
Relative Source Contribution (RSC)	20%	Fraction of total exposure attributable to freshwater/ estuarine fish	For most chemicals, available data support a larger RSC	Larger RSC yields 1.5x to 4x higher HHAWQC
Body Weight (BW)	70 kg	Adult weight, average for the general population	Mean body weight for adults is now 80 kg	Use of 80 kg yields 1.125x higher HHAWQC
Drinking Water Intake (DI)	2 L/day	86^{th} percentile of general population	Assumes all water consumed is at HHAWQC and that all drinking water is untreated surface water	Magnitude is compound specific[7]
Fish Intake (FI)	17.5 grams/ day for general population and sportfishers 142.4 grams/ day for subsistence fishers	90th percentile per capita consumption rate for the U.S. adult population	Represents an upper percentile, most people eat less fish	Magnitude is compound specific[8]
Bioconcentration Factor (BCF)	Substance specific	Tissue:water ratio at 3% tissue lipid	NA	NA

[7] HHAQWC are inversely proportional to DI value for substances with low BCFs. The DI value has very little influence on HHAWQC for substances with high BCFs.

[8] HHAQWC are inversely proportional to FI value for substances with high BCFs. The FI value has very little influence on HHAWQC for substances with low BCFs.

Table 6.10 Conservatism in Implicit Exposure Parameters

Implicit Exposure Parameter	Default Value	Represents:	Default is conservative because:	Impact of conservatism on HHAWQC (if known)
Cooking Loss	zero	loss of organic chemical during cooking	Does not account for the known 20-50% reduction in concentration of organic chemical in fish tissues following cooking	Inclusion of a factor to account for cooking loss yields 1.25x to 2x higher HHAWQC
Exposure Duration	70 years	Length of time a person is exposed	Assumes 100% of drinking water and fish consumed over the course of 70 years will come from a regulated water body	For non-ubiquitous compounds, recognizing that residency periods are much shorter than 70 years yields HHAQWC that are 2x to 8x higher.
Exposure Concentration	HHAWQC	Concentration in water body of interest equal to HHAWQC	Assumes concentration is always equal to HHAWQC without regard for changes in input or in flow characteristics	Magnitude uncertain but could easily be 1.5x to more than 4x
Relative Bioavailability	1	Bioavailability from fish and water compared to bioavailability in the experiment from which the toxicity benchmark was derived.	Some chemicals are less bioavailable in water or fish tissue than in the experiments from which toxicity benchmarks were derived.	Magnitude is chemical specific

7.0 IMPLICATIONS OF HHAWQC FOR FISH TISSUE CONCENTRATIONS AND CHEMICAL EXPOSURES VIA FISH CONSUMPTION

7.1 Fish Tissue Concentrations

The purpose for including factors for fish intake and bioaccumulation/bioconcentration in the derivation of HHAWQC is to account for consumption of chemicals that are contained within fish tissues. An underlying assumption of this approach is that the HHAWQC correspond to a chemical concentration in edible fish tissue that yields an acceptable daily intake when fish from surface waters

are consumed at the default intake rates (e.g., 17.5 g/day general population or 142 g/day subsistence anglers). Once a HHAWQC is calculated, the allowable fish tissue concentration (FTC) associated with that HHAWQC can be easily derived using the same equation. One way of assessing the overall conservatism of the process through which HHAWQC are derived is to compare the associated allowable fish tissue concentrations to existing fish tissue concentration data and concentrations found in other foods, as well as other guidelines or risk-based levels used to regulate chemical concentrations in edible fish tissues (e.g., fish consumption advisory "trigger levels," US Food and Drug Administration (FDA) tolerances).

Appendix C, "Fish Tissue Concentrations Allowed by USEPA Ambient Water Quality Criteria (AWQC): A Comparison with Other Regulatory Mechanisms Controlling Chemicals in Fish," illustrates this type of analysis using six example compounds: arsenic, methyl bromide, mercury (total, inorganic, organic), PCBS (total), chlordane, and bis-(2-ethylhexyl)phthalate (BEHP). The analysis revealed that:

- Concentrations of PCBs and mercury in fish from virtually all surface waters in the U.S. exceed FTCs associated with HHAWQC derived using the FI rate for subsistence anglers (142 g/day).
- FTCs associated with HHAWQC derived using the FI rate for the general public (17.5 g/day) are 20 times to 4,000 times lower (more stringent) than fish consumption advisory "trigger levels" commonly used by state programs.
- Although about 50% of fish samples collected during a national survey had PCB levels greater than the allowable PCB FTC associated with the HHAWQC, only about 15% of the nation's reservoirs and lakes (on a surface area basis) are subject to a fish consumption advisory. When the FI for subsistence anglers is used to calculate a HHAWQC for PCBs, the percentage of samples exceeding the associated FTC increases to 95%.
- The FDA food tolerances for PCBs, chlordane, and mercury in fish are, respectively, 500, 27, and 2.5 times greater than the FTCs associated with the HHAWQC for those chemicals. If the subsistence angler FI rate (142 g/day) is used to calculate the HHAWQC, the FDA food tolerances for those chemicals are, respectively, 4,000, 214, and 20 times greater.

These results indicate that, with respect to FTCs, the HHAWQC as they are currently calculated, with a default FI rate of 17.5 g/day, provides a wide margin of safety below the FTCs considered acceptable by states (as indicated by FCA trigger levels) and by the FDA (as indicated by food tolerances).

7.2 Chemical Exposures via Fish Consumption

Once the FTC associated with a HHAWQC is calculated, that value can also be used to estimate the allowable daily dose of that chemical. Comparing the allowable daily dose associated with HHAWQC with actual exposures to the general population via other sources provides an indication of the potential health benefits that might be gained by increasing the default fish consumption rate and thus lowering the HHAWQC. Appendix C shows the results of such a comparison for six example compounds (arsenic, methyl bromide, mercury (total, inorganic, organic), PCBS (total), chlordane, and BEHP and indicates that for all of these chemicals, exposure via consumption of fish from surface waters to which HHAWQC apply represents only a small percentage of the total exposure from all sources. Therefore, reducing exposures to chemicals via fish consumption by lowering HHAWQC may not provide any measurable health benefits.

8.0 CONCLUSIONS

HHAWQC are derived by EPA, or by authorized states or tribes, under the authority of Section 304(a) (1) of the Clean Water Act (CWA). The methodology by which HHAWQC are derived is based on equations that express a risk analysis. The values used in the HHAWQC equation are based on scientific observations (generally a range of observations) and, thus, have a scientific basis. However, the selection of a single value to represent the full range of observations represents a policy choice and is a subjective decision. Therefore, HHAWQC, though based on science, represent a policy (i.e., non-scientific) choice (EPA 2011a). EPA has stated that their goal in setting HHAWQC is to "protect individuals who represent high-end exposures (typically around the 90th percentile and above) or those who have some underlying biological sensitivity" (EPA 2004). To that end, its selections for individual default parameter values are typically upper percentiles of a distribution (e.g., a 90th percentiles value for fish consumption rate) or conservative assumptions (e.g., 100% of water used for drinking and cooking during a 70 year lifespan is untreated surface water).

The parameters used in the derivation of HHAWQC may be divided into two categories, toxicity parameters and exposure parameters. Toxicity parameters fall into three categories: 1.) non-carcinogenic effects, for which the parameter is the RfD, 2.) non-linear carcinogenic effects, for which the parameters are the POD and UF, and 3.) linear carcinogenic effects, for which the parameter is the RSD, which is derived from the slope factor and the target incremental cancer risk. Derivation of an RfD, selection of a POD and UFs, modeling the dose-response for carcinogenic effects, and calculating the slope factor (m) are based on science, but also involve a variety of policy decisions. These policy decisions all embody some degree of conservatism, such as the use of multiple 95th percentiles and upper bound confidence limits. Thus, the factors representing toxicity in the HHAWQC derivation equation certainly represent conservative (i.e., selected to more likely overestimate than underestimate risks) estimates of toxicity and act to drive HHAWQC toward lower concentrations.

Explicit exposure parameters include the RSC, BW, DI, FI, and BAF. There are also implicit parameters that, while not components of the equations used to calculate HHAWQC, are assumptions that underlie HHAWQC derivation. As with the toxicity parameters, most of the exposure parameters are based on scientific observations, generally a range of observations and thus have a scientific basis. However, selection of a single value to represent the full range of observations is a policy choice. Default values for these parameters and the degree of conservatism associated with them are summarized in Tables 6.9 and 6.10, which shows that these parameter values represent upper percentile values and highly conservative assumptions that act to drive HHAWQC toward lower concentrations.

EPA acknowledges in more recent guidance that the existence of the phenomenon of compounded conservatism, which occurs when the combination of multiple highly conservative assumptions leads to unrealistic estimates of risk. It suggests that in order to avoid this problem when constructing estimates from a series of factors (e.g., exposure and toxicity estimates), not all factors should be set to values that maximize exposure, dose, or effect (e.g., EPA 2005). However, in spite of that, most of the parameters used for the derivation of HHAWQC are set at the 90th (or higher) percentile level.

The overall level of conservatism embodied within the HHAWQC derivation process is illustrated by comparing the allowable fish tissue concentration implied by the designation of HHAWQC to existing guidelines or risk-based levels used to regulate chemical concentrations in edible fish tissues, such as fish consumption advisory "trigger levels" and US Food and Drug Administration (FDA) tolerances. Fish tissue concentrations associated with HHAWQC derived using the fish intake rate for the general public (17.5 g/day) are 20 times to 4,000 times lower (more stringent) than fish consumption advisory "trigger levels" commonly used by state programs. Similarly, FDA food tolerances for PCBs, chlordane, and mercury in fish are, respectively, 500, 27, and 2.5 times greater

than the HHAWQC-associated fish tissue concentrations and if the subsistence angler fish intake rate (142 g/day) is used to calculate the HHAWQC, the FDA food tolerances for those chemicals are, respectively, 4,000, 214, and 20 times greater.

Following a consideration of the overall level of conservatism contained within the HHAWQC, the level of protectiveness that EPA has indicated that states should achieve, and concerns that have been expressed by certain segments of the public and some state regulators and elected officials, three issues in particular seem to stand out. The first is the idea that HHAWQC represent an estimate of likely actual exposures to the public, such that, for example, if a HHAWQC is set at 42 ppb, the general public will be exposed to 42 ppb and therefore, any subgroups that may, e.g., consume more fish than average, will not be adequately protected by a 42 ppb HHAWQC. However, a consideration of the sources of the various parameters used to calculate the HHAWQC, as provided in preceding sections of this report, clearly shows that this is not the case.

The second is the idea that, because the HHAWQC for carcinogens are based on a 10^{-6} risk level for the general population, highly exposed subgroups whose risk level might be 10^{-5} or 10^{-4} are not being adequately protected. A consideration of the concept of population risk, as described in Section 6.1.3 demonstrates that this is not the case. Even if a small subgroup of the general population has higher exposures (e.g., higher rates of fish consumption), the expected number of excess cancers corresponding to individual risks at the 10^{-4} risk level is essentially zero. Indeed, in actual practice, in Federal regulatory decisions related to small population risks, the *de minimis* lifetime risk is typically considered to be 10^{-4}.

Finally, there is the belief that increasing the fish consumption rates used to derive HHAWQC which will, in turn, lower HHAWQC, will benefit public health, particularly for populations of high level consumers of fish from regulated surface waters. However, an analysis of six chemicals, selected to represent a range of chemical classes, clearly shows that exposures via consumption of fish from regulated water bodies is only a small percentage of the total dietary exposure from all sources. Thus, the establishment of more stringent HHAWQC may not provide any measurable public health benefit.

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APPENDIX A

FISH CONSUMPTION RATE (FCR)

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1.0 INTRODUCTION

A key component of the equation used to derive ambient water quality criteria (AWQC) is the long-term fish consumption rate (FCR). Selection of an appropriate FCR can be challenging for a number of reasons. In certain cases, there may not be relevant, local or regional fish consumption data available from which to select rates. In other instances, numerous studies of fish consumption behaviors may have been conducted, but the studies report a wide range of FCRs for similar consumer populations. Often, in light of the variability in FCRs, there is a tendency for regulators to select the most conservative (highest) of the available rates to ensure that HHAWQC will be protective of potentially exposed populations, thereby adding considerable conservative bias to the HHAWQC. While there is always variability in consumption rates due to differing behaviors among the consumers, in many cases, the variability among the reported rates for similar populations is a consequence of the survey design, methodology, and approach used to analyze the data, rather than actual variability in consumption rates. It is important to understand how the approaches used to collect and analyze fish consumption data may bias results so that the most appropriate and representative rates can be selected for the development of HHAWQC.

2.0 CURRENT EPA GUIDANCE

EPA's (2000) methodology for deriving AWQC recommends that, when available, consumption rates for populations of concern should be drawn from local or regional survey data. The consideration of local and regional survey data is important in deriving AWQC because these data may vary widely depending upon the waterbodies to which the AWQC will be applied, the population of individuals who may consume fish from those waterbodies, seasonal influences on fishing, availability of desirable species, and the particular consumption habits of those individuals. In many situations, the population of consumers may be the general population who consume fish from commercial sources; in other situations, the only consumers may be the population of fishermen who catch and consume their own fish from a particular waterbody. Typically, recreational fishermen are the population that is likely to consume the most fish from a specific waterbody as they may repeatedly fish that waterbody over time. This is a common rationale for using the habits of this population as a basis for deriving an FCR to be used in developing AWQC.

When local or regional survey data are not available, EPA has historically recommended that a default FCR of 17.5 g/day be used (EPA 2000). This rate is an estimate of the 90th percentile rate of consumption of freshwater and estuarine finfish and shellfish by adults in the general population of the United States. It is an annualized, long-term rate that indicates that the targeted population may consume roughly one half-pound fish meal every two weeks (28 meals/year) from the waterbodies to which the AWQC will be applied. It is based on the USDA's Continuing Food Studies data (USDA 1998) and is recommended by EPA for deriving AWQC because it represents an estimate of high end fish consumption by the general population and average consumption among sport anglers. If subsistence populations are present, EPA (2000) states that a default consumption rate of 142.4 g/day may be used. This rate indicates that this population may consume roughly 229 half-pound meals of fish per year or more than four meals per week.

In addition, EPA (2011) has evaluated a substantial portion of the fish consumption literature and has presented the results of its analysis in its revised *Exposure Factors Handbook*. This guidance presents

the findings of the studies and the estimates that EPA has derived based on its analysis of the data. A variety of recommended FCRs are presented for the general population of the United States, individuals who consume sport-caught fish from marine waters, individuals who consume sport-caught fish from freshwaters, and various subpopulations of fishermen. While the previous version of the *Exposure Factors Handbook* made specific recommendations of FCRs to be used, the revised version does not provide specific recommendations. Instead, it presents a range of values from studies that it identified as being relevant and reliable and instructs readers to select the value that is most relevant to their needs.

One difficulty with the way that the FCRs are presented in EPA's tables of recommendations is that not all studies are conducted in the same way. While the text of that guidance discusses the methodologies, strengths and weaknesses of each of those studies, it presents the resulting rates as if they are equivalent. However, the choices made in study design, target population, and approach to data analysis result in a wide range of FCRs. This variability among the FCRs presented can be confusing, resulting in a tendency for risk managers to select rates at the high end of those ranges to ensure protection of public health. The variability, however, is primarily the result of differences in the types of populations and fisheries studied, and the study designs employed. It is important to consider all of these factors in selecting an FCR (Ebert et al. 1994). When setting AWQC, it is important to select values that are representative of the target population to ensure that public health is being protected without putting unmanageable or unnecessary burdens on those who must comply with the AWQC (Ebert et al. 1994).

3.0 ANALYSIS OF FCR SURVEY DATA

While there are many studies of fishing consumption behavior available, it is important to consider the quality of the studies for the purpose of estimating FCRs. Many fishing surveys include collection of some data related to consumption of fish but often that is not the purpose for which the surveys were designed. Instead they may have been designed to determine dietary preferences, assess compliance with advisories, estimate fishing effort and success, determine angler preferences, etc. As such, while they may contain some information about consumption by the surveyed individuals, the data collected may not be adequately detailed or comprehensive to permit the estimation of reliable, long-term FCRs for that population.

For example, Connelly et al. (1992) conducted a survey of New York recreational anglers that provided information about sport-caught fish consumption but the study was designed for the purpose of providing information about anglers' knowledge of fishing advisories in New York and the impacts of the advisories on their fishing and consumption behavior. While it collected information about the number of meals and species consumed, it did not collect information about the size of fish meals. In order to use these data, one must make an assumption about the size of each meal, which in turn affects the rates derived from the study. When EPA (2011) analyzed these data to derive consumption rates, they assumed that each meal was 150 g in size based on a study of the general population conducted by Pao et al. (1982). Had EPA made different assumptions about meal size, they might have derived substantially higher or lower consumption rate estimates. It cannot be determined from the available data whether the rates derived by EPA were actually representative of consumption rates for the surveyed population.

There are a number of other survey design and analysis issues that affect the estimation of FCRs that may be considered in deriving AWQC. To better understand the nuances of FCRs derived from surveys of target populations, it is important to understand the influence that survey design and analysis can have on consumption rate estimates. These issues are discussed below.

3.1 Survey Methods

Fish consumption surveys can be conducted in a number of different ways. These methods include creel (or intercept) surveys, recall mail and telephone surveys, fishing diaries, and dietary recall studies. Each of these methods can be designed to provide information based on short- or long-term periods of recall (periods of time over which individuals are asked to remember their fish consumption behaviors).

While each of the survey methods can be used to estimate rates of consumption, each method has particular strengths and weaknesses and the survey design can greatly affect the resulting FCR estimates. Thus, the survey method used, the recall period, and the target population all need to be considered carefully when comparing FCRs that are reported. Many times the magnitude of the estimated FCRs are an artifact of the study methodology rather than a reflection of actual differences in fish consumption behaviors.

3.1.1 Creel Surveys

Historically, creel surveys have been used by fisheries managers to collect information about catch and harvest rates and determine the adequacy and characteristics of fishery stock. In some cases, however, creel surveys are modified to collect specific information about fish consumption based on individual fishing trips to a particular waterbody. Generally, survey clerks make contact with individuals who are fishing on a particular survey day to ask them what they have caught and what they intend to eat. Typically individuals are only interviewed once during a survey period (no repeat interview) although sometimes repeat interviews are part of the survey design and the responses on multiple interview days are combined for the individual.

Creel surveys are very effective for collecting information about consumption from a specific waterbody by the individuals who use that waterbody. In addition, if there is a particular subpopulation that uses the fishery differently from the general angler population, those individuals will be identified and their consumption habits captured.

While creel surveys provide reliable information about the fish catch on the day of the interview, they are subject to a number of limitations when attempting to estimate long-term average FCRs, which are the rates that are generally used in developing AWQC.

- Consumption rates based on creel surveys are subject to avidity bias; that is, there is a greater chance of interviewing more avid anglers because they are present at the fishery more frequently. More avid anglers are likely to be more successful anglers and, if they harvest fish for consumption, their rates of consumption are likely to be higher than the typical anglers' consumption rates. In order to use creel survey data to estimate consumption habits of the total user population, it is necessary to make a correction for avidity bias so that the results are representative of the entire angler population that uses the fishery (EPA 2011).

  EPA (2011) discusses this phenomenon in its discussion of FCRs in its 2011 *Exposure Factors Handbook*, stating that "in a creel study, the target population is anyone who fishes at the locations being studied. Generally in a creel study, the probability of being sampled is not the same for all members of the target population. For instance, if the survey is conducted for one day at a site, then it will include all persons who fish there daily but only about 1/7 of the people who fish there weekly, $1/30^{th}$ of the people who fish there monthly, etc. In this example, the probability of being sampled … is seen to be proportional to the frequency of fishing...[B]ecause the sampling probabilities in a creel survey, even with repeated interviewing at a site, are highly dependent on fishing frequency, the fish intake distributions reported for these surveys are not reflective of the corresponding target populations. Instead, those individuals with high fishing frequencies are given too big a weight and the distribution

is skewed to the right, i.e., it overestimates the target population distribution." (EPA 2011, p. 10-3)

To correct for avidity bias, the survey sample is typically weighted based on the reported frequency of fishing by survey participants (EPA 2011; Price et al. 1994). For example, a single day of surveying may have encountered three individuals: 1) one individual who fished with a frequency of one day per year; 2) one individual who fished with a frequency of one day per month; and 3) one individual who fished daily. If those individuals ate one half pound (227 g) fish meal on each day of fishing, their annualized average daily FCRs would be 0.62, 7.5 and 227 g/day, respectively. Based on this 3-person sample, one would conclude that the average consumption rate for these three individuals was 78 g/day. However, if the survey were to be conducted at that location daily throughout the year, it is likely that it might have encountered 365 individuals who fished once per year, 12 individuals who fished once per month, and one individual who fished daily. Thus, the total user population would be 396 individuals, representing 396 points on the fish consumption distribution for the total user population. If their FCRs were identical to the rates for the individuals interviewed during the single day of the survey, the result would be 365 individuals consuming 0.62 g/day, 30 individuals consuming 7.5 g/day, and 1 individual consuming 227 g/day. Thus, for this total angler population, the average rate would be 1.7 g/day. This is substantially lower than the average of 78 g/day based on the actual sample of three individuals. This demonstrates the considerable conservative bias introduced to the FCR estimate if avidity bias is not corrected. Actual corrections depend on the frequency of sampling and the population sampled and so need to be made on a study-by-study basis.

While it is now recognized that avidity bias needs to be considered when analyzing survey data to derive estimates that are representative of the total consuming population, this was not generally done for historical surveys and is still often not done by current study authors. Instead, the consumption rates presented in many survey reports reflect the consumption rates derived from only those individuals who were sampled and thus are biased toward more frequent anglers and consumers. Sometimes it is possible to make these corrections retroactively if the raw data are still available, but often this is not the case. As a result, many consumption estimates that are presented based on creel survey data have not been adjusted to reduce this conservative bias and consequently overestimate consumption rates for the total target population.

- Short-term behavior captured during a single snapshot in time may not be representative of long-term behavior because of variability in fishing effort and success. There may be substantial seasonal variations in the habits of anglers due to fishing regulations, climate, and the availability of target species. Consequently, information collected during a single interview may not be representative of activity on previous or subsequent trips or at other times of the year. Because of limited time for conducting interviews, it is difficult to ask enough detailed questions to allow development of a reliable estimate of the long-term rates of consumption. In addition, the assumptions that must generally be made to extrapolate from short-term data to estimate long-term behaviors add greatly to the uncertainties associated with those estimates.

  Creel surveys are effective at characterizing the consumption habits of individuals who use a specific fishery and are helpful in identifying any subpopulations of fish consumers that are present. It is more challenging, however, to derive a long-term estimate of consumption or to expand the results to a larger geographic area unless very detailed information is collected and there is an appropriate correction for avidity bias.

3.1.2 *Mail Surveys*

Mail surveys are a good tool for collecting detailed information about fishing and consumption behaviors. Generally, mail surveys are designed to randomly sample the target population. Often, for

fish consumption, the target population is recreational anglers and mailing addresses are obtained from fishing licenses sold within the target area. Mail surveys can generally collect more detailed information over a longer period of recall, ranging from months to a year. There are, however, some limitations associated with the use of mail surveys.

- Response rates may be low, unless there is a concerted follow-up effort. If rates are very low, then the resulting FCRs may not be representative of the entire target population. In this case, rates are generally overestimated due to the fact that individuals who choose to respond to the survey tend to self-select; that is, the individuals who are most likely to return a mail survey are those for which fishing is an important activity. These individuals tend to be more avid anglers who fish more frequently than the typical angler population and have a higher rate of success in catching fish. Thus, consumption rates based on data collected in a survey with a low response rate may be biased higher than rates that would be estimated if the entire angler population was equally represented in the survey data.

- Because mail surveys often focus on a longer period of recall, the resulting FCRs are subject to recall bias. It is possible that difficulties in recalling specific information about fishing activity may result in the omission of some meals; however, data on the biases associated with long-term recall periods for recreational activities indicate that individuals tend to overestimate their participation, particularly if the issue being investigated is salient for them (Westat 1989). Thus, the tendency is for FCRs to be overestimated with longer recall periods.

- It can be difficult to target certain subpopulations of fish consumers (e.g., high end consumers, specific ethnic groups, individuals who fish a particular waterbody, etc.) with a mail survey. Individuals who are homeless or migrant will not be captured, and those individuals who have limited language skills and/or low levels of literacy may not understand the survey questions and, thus, may choose not to complete and return it. Thus, these groups may be under-represented in the survey sample.

Mail surveys are often conducted to collect information on a statewide or regional basis. If well designed, they can provide detailed information about the fish consumption behaviors of study participants as they can be completed at the respondent's leisure rather than requiring instantaneous recall of past events. However, FCRs derived from mail surveys may be overestimated if recall periods are long. They may also be overestimated if response rates are low because often non-respondents are less interested in the subject of the survey and, therefore, choose not to participate. In this case, however, data collected through follow-up contact with non-respondents can be used to adjust survey results.

3.1.3 *Telephone Surveys*

Telephone surveys generally consist of the one-time collection of data from a survey participant by telephone. Lists of telephone numbers of individuals within the target population are developed either through the random selection of telephone numbers from all telephone listings in a given area (e.g., statewide, population within certain counties, or population within certain zip codes near a specific waterbody or fishery) or, in the case of surveys of recreational anglers, may be based on information obtained from fishing licenses purchased. Survey respondents are asked to recall information about past fishing trips and fish consumption behavior.

Telephone surveys are rarely used in isolation, however, and are often a follow-up to surveys that have been previously sent to the targeted individuals, thereby providing an opportunity for those individuals to review the survey questions before being asked to respond to them (EPA 1992). They may also be conducted to provide information about non-response bias (for those individuals who did

not respond to a mail survey effort) or to confirm or add to data that were collected in the field during a creel survey (EPA 1992).

Telephone surveys are effective in evaluating regional information and can reach large numbers of individuals (EPA 1992) but also have limitations, including the following:

- Individuals who are being interviewed by telephone are rarely willing to spend more than 10 or 15 minutes participating in a telephone interview, particularly when they have had no warning that they will be called. This limits the amount of information that can be captured from them and is likely to result in recall bias due to the fact that individuals may not recall information completely or accurately when they are unprepared to do so. In addition, because of limited time, they can only be asked general information about their long-term fish consumption habits or specific information about their most recent activities.

- Because telephone surveys generally only include a single interview with an individual, they are subject to bias due to the fact that the responses of the participants may only reflect their most recent activities. Thus, if the telephone interview occurs at a time that the respondent is actively fishing or consuming fish, the resulting data may over-estimate his long term level of activity. At the same time, if the telephone interview occurs during a period of inactivity, his long term consumption activity may be under-estimated.

- Individuals who do not have telephones cannot be included in the sample population. Because those individuals are likely to be low income individuals who cannot afford the cost of a telephone, this segment of the population is likely to be under-represented in the survey sample. Similarly, individuals with unlisted numbers will not be included in the survey.

- Recent telephone surveys may be biased toward an older, higher income population if they have not included the sampling of cell phones in addition to land lines, as younger people are more likely than older individuals to rely completely on cell phones. In addition, even if cell phones are sampled, it is not always possible to accurately sample the geographic location targeted because cell phones are not tied to specific addresses (individuals may move to a different home or area but retain the same cell phone number).

- Telephone surveys can be useful if the general population of a given area is being targeted or if anglers are being targeted and the telephone numbers have been obtained from recent fishing licenses. However, if the target population is a particular socioeconomic subpopulation (e.g., ethnicity or income level), it is very difficult to identify those individuals in advance when selecting a list of telephone numbers. Thus, the smaller the target population, the larger the survey effort necessary to gain enough data about the subpopulation or group of interest.

All of these issues can affect the FCR estimates that are derived based on a telephone survey. The most important considerations are the way that the short-term recall information has been used to estimate long term consumption rates and the attention to avoiding the bias introduced in survey results if certain segments of the population are not well represented in the sampling.

3.1.4 *Fishing Diaries*

Diary studies are an excellent means of collecting detailed information about specific fishing trips and fish meals. In these studies, individuals from the targeted population are recruited to participate in the study and are asked to keep a diary of the fishing trips taken. These studies can be short- or long-term studies. For long-term studies, individuals are generally asked to complete monthly diaries and can record very detailed information about every trip taken and every harvested fish that was consumed. If the individuals complete the diaries in a timely fashion, these studies minimize the potential for

recall bias and also increase the level of detail that the person is able to recall (e.g., the size of a fish meal, the species consumed, the number of people who shared in the meal, etc.). If this information is collected over a long time period (e.g., for example, monthly diaries completed over a one year period), it can result in very accurate estimates of long-term fish consumption.

One difficulty with long-term diary studies is that there can be a high level of attrition because people tire of recording their information and so stop completing the diaries. However, while the information gathered may only be partial (e.g., several months of the targeted one-year period for the study), the level of detail provided in the diary and the partial data can still yield valid estimates of long-term fish consumption behaviors by the study participants (Balogh et al. 1971).

3.1.5 *Diet Recall Studies*

Diet recall studies are a form of diary study but are generally shorter term. In these studies, individuals are commonly asked to record all foods eaten during a one- or two-day period. The days may be consecutive days or two different days during the study period. These recall studies work well for foods that are consumed on a regular basis (i.e., foods that are consumed daily or at least once every two days) and when evaluating population-level trends, but are not as effective for developing reliable estimates of long-term consumption behavior of foods that are consumed less regularly (as discussed in more detail in Section 3.2.2)). Thus, for those individuals who consume fish daily or several times per week, the estimated rates of consumption based on these data may be representative of their behavior.

However, for many individuals, fish is not consumed on a daily or regular basis. This is particularly true of sport-caught fish, which may only be consumed occasionally (e.g., once per week or less or only during a specific time of the year) (Ebert et al. 1994). As discussed in more detail in Section 3.2.2, short-term recall periods may substantially bias the results by incorrectly assuming that individuals who did not consume during the recall period are non-consumers, and leaving them out of the consumption rate distribution, thereby skewing that distribution toward more frequent consumers. This results in overestimated consumption rates for the total population. In addition, the timing of the diet recall study can substantially affect the resulting consumption estimates if there is a seasonal component to the consumption habits of sport-fishermen. For example, in most states, fishing regulations limit the harvest for individual fish species to certain times of the year. Some individuals have a strong preference for a certain species and only consume fish when those species are available. Thus, while they may consume those fish regularly during that season, they may not consume fish at all during the remainder of the year. If the diet recall survey is conducted during the season when they are regularly consuming those fish, and the survey is not carefully designed to address seasonal variations, their annualized, average FCRs will be overestimated. Conversely, if the diet recall study is conducted during the time when these fish are not being consumed, their FCR will be underestimated as it will, by necessity (due to lack of consumption information) be assumed that they are non-consumers. Because of this, their consumption will not be included in the consumption rate distribution from the survey, thereby biasing that distribution to more frequent consumers and higher consumption rates.

3.2 Analysis of Survey Data to Derive FCRs

Data from surveys can be analyzed a number of different ways and the approach to analysis will depend, in part, on survey design. The key consumption metric for deriving AWQC is to derive an annualized average daily FCR. When estimating these FCRs, it is necessary to understand the size of each meal consumed and the frequency with which those meals are consumed.

There are two common approaches for estimating consumption rates. These include an approach based on reported meal frequency and size, and an approach based on the amount of fish harvested and consumed on a yearly basis.

The meal frequency approach requires that information on the number and size of meals consumed by the surveyed individual over a period of time be collected and then extrapolated to the extent necessary to derive an annualized daily average FCR. Thus, for example, if the survey respondent indicates that he or she eats 26 half-pound [227 gram (g)] fish meals per year, the ingestion rate would be calculated as follows:

FCR = 26 meals/yr * 227 g/meal * 1 yr/365 days = 16.2 g/day

Similarly, if the respondent indicates that she eats 1 meal every two weeks, her FCR is calculated as follows:

FCR = 0.5 meal/week * 227 g/meal * 52 weeks/year * 1 yr/365 days = 16.2 g/day

Alternatively, the harvest rate approach uses information about the mass of fish actually harvested by the survey participant over time, adjusts that mass by the edible portion of the fish (total mass minus the mass of the parts not consumed by the angler, such as viscera, head, bones, etc.) and the number of people to share in the fish meal. Thus, if a survey respondent indicates that he or she harvested 40 kg (88 pounds) of fish during a year, the default edible fraction of 30 percent (EPA 1989) is used, and it is reported that a total of 2 adults consumed the fish, the FCR would be calculated as follows:

FCR = 40,000 g whole fish/yr * 0.30 g edible/g whole * 1/2 persons * 1yr/365 days = 16.4 g/day

Depending upon the survey approach used and the questions asked, one method may be more appropriate than the other. There are some limitations of each of these approaches, however, that need to be considered.

- There are uncertainties about the meal method due to the fact that the size of fish meals may vary considerably. Meals of store-purchased fish are likely to be fairly consistent due to the fact that a consistent amount of fish may be purchased for consumption. The same is not true for sport-caught fish. Meal sizes will vary depending upon the mass of fish harvested on a given day and the number of individuals consuming it. Thus, because individuals are generally asked to estimate the size of fish meals consumed, they may or may not accurately represent the variety of meal sizes that are actually consumed over time if the fish are sport-caught fish. While individuals involved in the surveys are often provided with photographs of meals of different sizes, these estimated meal weights may not be representative of the fish actually consumed due to differences in mass resulting from cooking, the way the fish were prepared, and the density of the fish tissue. In addition, although they may provide their estimated average weekly rate of consumption, this weekly rate may vary considerably by season due to changes in weather, fishing time, or availability of target species. Unless data are collected to specifically capture these variations, there is substantial uncertainty introduced by this approach.

- There are also uncertainties introduced when using the harvest method because individuals may not recall exactly how much fish they have harvested over time, and the portion sizes of the individuals who share in the consumption of the fish may vary. Thus, if two people share in the catch it will normally be assumed that the total mass should be divided by two; however, the portions consumed by those individuals may not be equivalent. In addition, there may be some variability around the edible portion of the fish depending on the parts consumed by the survey participants, the fact that edible portions vary somewhat by species, and the number of individuals who share in individual fish meals.

3.2.1 *Identifying "Consumers" and "Non-Consumers"*

When determining the population to be targeted in selecting an FCR for use in developing AWQC, it is important to determine who is likely to be exposed to that chemical via the consumption of fish. Clearly, individuals who never consume fish will have no potential for exposure via this pathway so that the emphasis needs to be on the individuals who actually consume fish as this will be the potentially exposed population. However, depending upon the waterbodies to which the AWQC will be applied, the fish consuming population will vary. If the AWQC will be applied to waterbodies that are commercially fished, then there is potential for exposure to the general population, because they will have access to that fish through commercial sources such as fish markets, grocery stores and restaurants. However, if the waterbodies that are the focus of the AWQC are not commercially fished, then the fish from those waterbodies will not be available to the general population. The only sources of those fish are the recreational anglers who fish those waterbodies.

Once the target population has been identified, it is necessary to identify the FCRs for the individuals within that population who consume fish. Depending upon the survey approach used, this determination can be challenging. For example, if the AWQC are to be applied to commercially fished waterbodies, then the general population who have access to those fish is the target population. However, most surveys of the general population collect information about total fish consumption including consumption of fresh, frozen, canned and prepared fish and shellfish obtained from stores and restaurants, which are most often imported from locations outside of the area of influence of the AWQC, as well as sport-caught fish and shellfish from local sources.

Even if the survey has distinguished among different sources of fish, the identification of consumers may be affected by the survey method. As discussed in more detail in Section 3.2.2 below, short-term diet recall studies, which are often used to evaluate food consumption within the general population, often misclassify individuals as non-consumers. Thus, while the rates are reportedly based on consumers of those fish, they are likely to be excluding a large proportion of actual consumers who have lower frequency of consumption.

3.2.2 *Limitations on the Use of Short Recall Period Survey Data*

Attempting to extrapolate long-term FCRs based on short recall period survey data presents a number of problems. These include the potential misclassification of non-consumers, the overestimation of FCRs based on data collected as a snapshot in time, and the lack of consideration of variation over time.

In general, the length of recall period affects the resulting estimated rates of consumption with shorter term studies resulting in higher estimated rates of consumption than studies with longer recall periods. The higher rates of consumption from the short-term studies may not be a reflection of actual differences in the behaviors within the surveyed populations but may instead be an artifact of the short recall period (EPA 2011; Ebert et al. 1994).

Short-term dietary recall studies can result in misclassification of participants as non-consumers and consequently overestimate consumption rates for true consumers within the surveyed population. Essentially, when a diet recall survey is conducted, if an individual does not indicate that fish was consumed during the recall period, that individual is identified as a non-consumer and is assumed to have zero consumption. When this occurs, rates are reported as either "per capita" rates (which include the non-consumers and their estimated rates of 0 g/day) or as "consumers only" rates, which means that all of the individuals who did not consume fish during that period of time are excluded from the reported results and only those individuals who did consume fish during that period are counted in the consumption rates.

The USDA dietary data that form the basis for EPA's (2000) default FCR of 17.5 g/day were collected using a dietary recall study of survey participants during two non-consecutive 24-hour periods (EPA, 2000). Because of the way in which sampling was conducted, the actual fish consumption behaviors reported are strongly biased toward those respondents who consume fish with a high frequency. All of the individuals included as fish consumers in the USDA estimate consumed fish at least once during the 2-day sampling period. To use these data to estimate long-term consumption rates, EPA assumes that the consumption behavior that occurred during the 2-day period is the same as the consumption behavior that occurs throughout every other 2-day period during the year. Thus, if an individual reported eating one fish meal during the sampling period, the extrapolation used to estimate long-term consumption was the assumption that the individual continues to eat fish with a frequency of one meal every two days, or as many as 183 meals per year. If it is assumed that an individual eats one-half pound (227 g) of fish per meal, this results in a consumption rate of 114 g/day. However, the individual who consumed fish during that sampling period may not actually be a regular fish consumer. In fact, that fish meal could have been the only fish meal that the individual consumed in an entire year. Thus, that person's FCR would be substantially overestimated using this extrapolation method.

Conversely, individuals who did not consume fish during the 2-day sampling period were assumed to be non-consumers of fish, despite the fact that those individuals may simply have been fish consumers who coincidentally did not consume fish during the 2-day sampling period. Because there are no data upon which to base consumption estimates for these individuals, they were assumed to consume 0 g/day. However, they may in fact consume fish with a frequency ranging from as little as zero meals per year to as much as one meal per day (or even more than one meal per day) on all days except the two that USDA conducted the survey. As with the high consumers identified in the USDA database, there is no way to determine whether 0 g/day consumers are actually non-consumers or just individuals who did not consume fish during the 2-day survey period.

There can be enormous variability in the frequency of consumption of specific foods (Balogh et al. 1971; Garn et al. 1976), and the variability in the number of fish meals may be further enhanced by seasonal effects. For example, recreational fishermen in many states are only permitted to fish during certain months due to fishing regulations. Thus, it is possible that their sport-caught fish ingestion rates are substantially higher during the fishing season, when fresh fish are readily available, than they are during the remainder of the year. In addition, many anglers target specific species and only fish when those species are available. For example, many anglers in the Pacific Northwest target salmon, which are only available during their time-limited spawning runs. Thus, they may not fish at all or consume sport-caught fish during other times of the year when the salmon are not available.

Because of this phenomenon, there is a tendency, if only "consumers" are considered, for short-term recall surveys to report substantially higher FCRs than do surveys with longer periods of recall. This is well demonstrated in EPA's (2011) tables of relevant fish consumption studies. For example, when reviewing EPA's relevant studies of statewide[9] freshwater recreational fish intake (EPA 2011, Table 10-5), FCRs appear to be highly variable, with means for "consuming" anglers ranging from 5.8 to 53 g/day and 95th percentile (95th %ile) values ranging from 26 to 61 g/day.[10] However, one of those studies collected data from individuals on a single day (ADEM 1994), one involved a single interview but also included a 10-day dietary diary component (Balcom et al. 1999), one involved a 90-day recall period (Williams et al. 1999), one included a 7-day recall period but also collected some

[9] There are additional studies provided on EPA's table of relevant studies but those studies are waterbody specific and thus are not directly comparable with the statewide studies.

[10] 95th percentiles are not available for all studies listed in EPA's Table 10-5. For example, EPA reports the highest mean rates for studies conducted in Alabama and Connecticut but provides no 95th percentile values from those studies. Thus, those studies cannot be included in the comparison of 95th %ile rates.

information on seasonal variation for the remainder of the year (West et al. 1989), and the remainder of the studies collected data for a 1-year recall period. When the statewide studies are segregated by recall period, the bias toward higher consumption rates based on shorter recall periods is apparent, as shown below.

Rates for Sport-caught Freshwater Fish Consumption (Adult consumers) from Statewide Studies by Recall Period (Table 10-5, EPA 2011)

Recall Period	1-day		1-day interview and 10-day diary		90 day				1 year	
Metric	Mean	95th %ile	Mean	95th %ile	Mean	95th %ile	Mean	95th %ile	Mean	95th %ile
FCR (g/day)	53	NA	53	NA	20	61	14	39	5.8-14	26-43
Study	ADEM 1994		Balcom et al. 1999		Williams et al. 1999		West et al. 1989		Ebert et al. 1993; Benson et al. 2001, Connelly et al. 1996, Fiore et al. 1989	

NA: Not available. This value was not presented by EPA (2011)

[a]The West et al. 1989 study requested information about a 7 day recall period but also collected some information on variation in behavior during different seasons of the year which were used to estimate long-term FCRs.

[b]A subsequent West et al. (1993) study collected information for a 7-day recall period but collected no longer term information that could be used to annualize the rates. While the means from the 1989 and 1993 surveys were nearly identical, the 95th percentile for the 1993 study (78 g/day; EPA 1997) was substantially higher than the 95th percentile of 39 g/day that was derived from the 1989 survey data.

Consumption of sport-caught fish is likely to have a seasonal component, particularly in states where fishing may occur for only a portion of the year. Like other seasonal foods, it is likely that these foods are eaten more frequently during their seasons than they are at other times of the year. For example, fresh, local strawberries are only available in the northeastern United States for a few weeks during the summer. When they are available locally, it is likely that strawberries are consumed in greater quantities than they are when they are out of season and can only be imported from other locations and purchased from supermarkets. That is not to say that they are never eaten when they are out of season but rather that if individuals were to be asked about their strawberry consumption during the time that fresh strawberries are in-season, it is likely that they would overestimate their consumption for other times of the year when local strawberries are not available. At the same time, if they were asked in the winter to report their strawberry consumption, it is likely that they would underestimate their strawberry consumption during the summer when fresh, local strawberries are readily available. These seasonal variations are important in terms of their affect on estimating long term consumption rates. While the USDA survey (upon which EPA's rate of 17.5 g/day is based) collected data on two different days, the survey days were no more than 10 days apart. Thus, the rates of consumption for all foods that are seasonally affected would have been dependent upon the timing of those survey days and would not necessarily reflect the participants' long-term average consumption rates.

EPA (2011) has acknowledged that short-term dietary records are problematic when attempting to estimate long-term rates of consumption, particularly for upper bound FCR estimates. In its review of NHANES 2003-2006 study data, EPA (2011, p. 10-16) stated, "the distribution of average daily intake rates generated using short-term data (e.g., 2-day) does not necessarily reflect the long-term distribution of average daily intake rates." In addition, in its discussion of the limitation of the West et al. (1993) study of Michigan anglers EPA (2011, p. 10-38) stated: "However, because this survey

only measured fish consumption over a short (1 week) interval, the resulting distribution will not be indicative of the long-term fish consumption distribution, and the upper percentiles reported from the U.S. EPA analysis will likely considerably overestimate the corresponding long-term percentiles. The overall 95th percentile calculated by U.S. EPA (1995) was 77.9; this is about double the 95th percentile estimated using yearlong consumption data from the 1989 Michigan survey." In addition, when discussing the USDA methodology, EPA (1998, p. 10-107) stated that "[t]he non-consumption of finfish or shellfish by a majority of individuals, combined with consumption data from high-end consumers, resulted in a wide range of observed fish consumption. This range of fish consumption data would tend to produce distributions of fish consumption with larger variances than would be associated with a longer survey period, such as 30 days." As a result, upper-bound fish consumption estimates based on these data will be biased high and overestimate actual upper-bound consumption rates for the total population of consumers.

Short-term recall periods generally result in an overestimate of consumption behavior, particularly for foods that are not eaten on a daily basis. While this does not appear to greatly affect central tendency values for the populations studied (EPA 2011; Garn et al. 1976), the inverse relationship between upper-bound FCRs and the length of survey recall period has been clearly demonstrated (Ebert et al. 1994).

3.2.3 *Estimating Means and Upper Percentiles*

Once FCRs have been calculated for the individual survey respondents, they are typically evaluated statistically to define a central tendency or upper-bound estimate of consumption to be used in deriving AWQC. The central tendency may be an arithmetic mean, geometric mean, or a median (50th percentile value) of the range of consumption rates derived. Because the estimated FCR distribution (the range of rates) is generally very highly skewed, as are consumption rates for most foods (Garn et al. 1976), with a very large number of individuals consuming fish at very low FCRs and a few individuals consuming at high rates, the arithmetic mean is typically not a good estimate of actual central tendency. For example, in the statewide survey of Maine's recreational anglers, which included rates ranging from 0.02 to 183 g/day, the median rate of consumption by individuals who ate at least one fish meal from Maine's freshwater bodies during the year was 2 g/day but the arithmetic mean FCR for this same population was 6.4 g/day and represented the 77th percentile of the distribution of FCRs from that survey (Ebert et al. 1993).

Upper-bound FCRs may be calculated in a number of ways. For some surveys, they may be calculated as the 95th upper confidence limit of the arithmetic mean consumption rate. Alternatively, for some surveys, FCR results are ranked in order of magnitude and then the upper-bound value is selected as the 95th percentile of that distribution. Thus, for example, in the same Maine survey for which there were 1,053 FCRs calculated, the 95th percentile value of 26 g/day represented the FCR reported for angler 1,000 after order ranking of the results (Ebert et al., 1993).

3.2.4 *Consumption of Resident and Anadromous Fish Species*

It is important that the FCR used in deriving AWQC reflects consumption of the fish species that will be affected by the AWQC. This will ensure that FCRs are not overestimated.

Estimated FCRs are generally based on the total consumption of fish, and may include fish of a variety of types, including resident finfish, anadromous finfish, and shellfish. For example, the FCR recently adopted by Oregon Department of Environmental Quality was supported by state-specific data on consumption for which a substantial portion of the consumption was the ingestion of anadromous species such as salmon and steelhead. Anadromous species are not substantially affected by local water quality in estuaries and rivers because they are only present in those waterbodies when they are juveniles and when they return as adults to spawn. They spend the majority of their lives in

marine waters and are typically harvested during their return spawning runs. As a result, any chemical constituents that are present in their bodies are predominantly the result of exposures they have received during their time in marine waters. Thus, changes in AWQC for local waterbodies will not affect the concentrations of those chemicals in their edible tissues. Instead the fish that are sensitive to changes in local water quality are the resident species that spend their entire life stages in local waters.

This is an important consideration for states, such as Oregon and Washington, where a substantial portion of the fish harvested for consumption are anadromous fish. For example, the Columbia River tribes consume, on average, nearly three times more anadromous fish (including salmon, trout, lamprey and smelt) as they do resident species (CRITFC 1994). Similarly, Toy et al. (1996) reported that at the 95th %ile consumption rate for the combined Tulalip and Squaxin tribes, who fish Puget Sound, 95% of the total finfish consumed were anadromous species.

Because the AWQC approach incorporates a chemical-specific bioaccumulation factor, it essentially assumes that fish are in equilibrium with constituent concentrations in the water bodies of interest. This is not likely to be the case for anadromous species because of the short time period during which they are in fresh and estuarine waters. For example, after hatching, juvenile Chinook salmon spend several months in the Columbia River before they begin their out-migration to marine feeding areas. They generally return to the river to spawn between the ages of two and six years (ODFW, 1989) and do not generally feed during their spawning run. These fish, which provide a substantial portion of the freshwater fish harvested both commercially and recreationally from the river, are clearly not at equilibrium with their surroundings.

Because migrating fish do not spend adequate time in a particular river reach to achieve equilibrium with concentrations in the water column and sediments there, the bioaccumulation factor used in developing the AWQC overestimates the tissue concentrations in such fish that can be attributed to that reach. It is only the resident species that will be impacted by local water quality. Consequently, the use of an FCR that includes anadromous fish substantially overestimates exposure to local chemicals. For example, if an individual has a total FCR of 20 g/day and 90 percent of the fish consumed during the year are anadromous fish, only 10 percent of the fish consumed, or 2 g/day, are resident fish that are likely to be affected by changes in local water quality. Thus, to use a total FCR of 20 g/day overestimates the individuals' actual potential for exposure due to local contaminants by a factor of 10. Instead, it is the consumption rates for resident species that should be used to derive AWQC because it is these species that will be affected by changes in water quality.

Not all states have the type of access to anadromous species that occurs in the Pacific Northwest. Thus, these fish will not constitute a substantial fraction of consumers' diets in many areas of the country. This makes it extremely important to ensure that the FCRs that are used in developing AWQC for a specific region are based on fish consumption information for that region and not simply based on a one-size-fits-all approach for selecting consumption rates.

3.2.5 *Consumption of Freshwater and Estuarine Species*

In developing AWQC in coastal states, the FCRs that are used typically do not differentiate between the ingestion of freshwater and estuarine finfish and shellfish. This is because AWQC need to be applied to a number of different types of water bodies. However, this assumption is very conservative when one considers permitting of individual discharges that occur in specific areas of individual water bodies and may only affect freshwater areas. If there is a permitted discharge to a freshwater body, the consumption of estuarine fish and shellfish is likely to be irrelevant. Similarly, if there is a discharge to an estuarine area, the freshwater fish upstream will likely not be affected by that discharge. Thus, inclusion of rates of consumption of freshwater and estuarine finfish and shellfish is

a very conservative assumption for these specific applications, providing an additional level of health protection when AWQC are applied to specific waterbodies.

4.0 POPULATION RISK

AWQC are typically derived using a target individual risk level of 1 in 1,000,000 million (1E-06) risk for carcinogens and a hazard index of 1 for non-carcinogens. For carcinogens, this target risk represents the increased probability that an individual will develop cancer as a result of exposure through the consumption of fish tissue. The background rate for contracting cancer is roughly 30 percent; thus, when a 1E-06 risk level is selected as the target risk, this means that the probability of an individual contracting cancer increases from 30 percent to 30.0001 percent.

There is, however, another risk metric that should be considered in selecting an FCR. This risk metric is known as the population risk. It is calculated by multiplying the target risk level by the size of the affected population to predict the number of excess cancer cases that might result from that exposure. Thus, if the target risk is 1 in one million, and the size of the population is one million people, the population risk will be calculated as 1 excess cancer over the combined lifetimes of 1 million individuals who are actually exposed as a result of the modeled exposures.

Population risk is an important consideration in selecting an FCR for use in developing AWQC because as the size of the exposed population decreases, the population risks also decrease when the same target risk level is used. The higher the FCR selected for a particular population, the smaller the population to which that FCR applies. For example, if the FCR selected is a 95^{th} percentile rate, it is assumed that it is protective of all but 5 percent of the exposed population or 50,000 of the 1 million people provided in the example above. Thus, if the same target risk level of 1E-06 is used with this reduced population, the resulting population risk is 0.05 excess cancers within a population of 1 million people. In other words, in order to reach the target risk of 1 excess cancer, it would be necessary for a population of 20 million people to have lifetime exposures equivalent to the estimated exposure conditions.

EPA (2000) states that both a 1E-06 and 1 in 100,000 (1E-05) target risk level may be acceptable for the general population as long as highly exposed populations do not exceed a target risk level of 1E-04 or 1 in 10,000. In other words, if an AWQC is based on a 1E-06 risk level and an FCR if 17.5 g/day is used, this means that if there is a subpopulation of individuals who consume fish at a rate of 175 g/day, they will be protected at a risk level of 1E-05, and in order for a subpopulation to exceed the recommended upper bound risk level of 1E-04 outlined in EPA's (2000) methodology, they would have to consume more than 1,750 g of fish daily throughout their lifetimes.

EPA (2000) states that "[a]doption of a 10-6 or 10-5 risk level, both of which States and authorized Tribes have chosen in adopting water quality standards to date, represents a generally acceptable risk management decision, and EPA intends to continue providing this flexibility to States and Tribes. EPA believes that such State or Tribal decisions are consistent with Section 303(c) if the State or authorized Tribe has identified the most highly exposed subpopulation, has demonstrated that the chosen risk level is adequately protective of the most highly exposed subpopulation, and has completed all necessary public participation" (EPA 2000).

Selection of an FCR to be used in developing AWQC is as much a policy decision as a technical decision. There are wide ranges of FCRs available depending upon the population targeted for study and it is important that the target population be identified so that the selection of an FCR rate can be based on that target population and the target risk level can consider both individual and population risks for that population.

5.0 DISCUSSION

When selecting an FCR for establishing HHAWQC, it is critical that a number of important issues be considered. These include: 1) identifying the target population of fish consumers and the waterbodies that will be affected by changes in HHAWQC; 2) evaluating and selecting FCRs based on fish consumption studies that provide reliable, long-term information on the fish consumption habits of the target populations and waterbodies; and 3) consideration of both individual and population risks in selecting an FCR.

Generally speaking, the population of interest for the development of HHAWQC consists of those individuals who consume freshwater or estuarine finfish and/or shellfish from the area of interest. If the waters to which HHAWQC are to be applied are commercially fished, then this population will include members of the general population who may consume fish from a wide variety of commercial and recreational sources. In this case, FCRs should be based on general population studies of good quality. If, however, the waterbodies of interest are not commercially fished, then the target population includes those anglers who catch and consume their own fish from those waterbodies and the FCR should be selected from regionally-appropriate studies of consumption by recreational anglers.

HHAWQC are used as environmental benchmarks and as objectives in the development of environmental permits. While they are applicable to all ambient waters in a state, they are most often considered for individual water bodies when state regulatory agencies are developing permitting and effluent limits. Thus, assumptions that are already judged and selected to be conservative when one is attempting to develop statewide criteria, become extremely conservative when considering individual water bodies.

In light of the way in which HHAWQC are applied in permitting, the approach used to develop HHAWQC includes a number of highly conservative assumptions, particularly for constituents that are limited and localized. The conservative assumptions used in the development of HHAWQC and subsequently applied to permitting typically include:

- FCRs that include the combined consumption of freshwater and estuarine fish and shellfish and, in some areas, include anadromous species that are not impacted by local water quality conditions;
- 100 percent of the fish consumed in a lifetime are obtained from a single, impacted waterbody;
- There is no reduction in chemical concentration that occurs as a result of cooking or preparation methods;
- Concentrations of compounds in fish are in equilibrium with compound concentrations in the water body; and,
- The allowable risk level upon which they are typically based is one in one million. This means that the probability of developing cancer over a lifetime increases from 30% to 30.0001%.

There are a very small number of individuals, if any, to whom all of these conservative assumptions would apply.

EPA's recommended FCR of 17.5 g/day can reasonable be judged as conservative and protective when used in establishing AWQC for a number of reasons.

- It is based on survey data collected by the USDA, which are surveys of the general population, and includes information about many species and meals of fish that would not be found in the waterbodies that are subject to the HHAWQC. The reported fish meals were obtained from numerous sources and included fresh, frozen, prepared and canned fish products that may have been produced in other regions of the United States or other countries and, consequently, not derived from local waterbodies. Thus, the USDA data overestimate the consumption of locally caught fish, particularly if there are no commercial fisheries, and certainly overstate consumption from individual waterbodies that are regulated under the HHAWQC.
- As discussed previously, this rate is based on 24-hour dietary recall data. Use of such data to estimate long term consumption rates for any population results in biased and highly uncertain estimates.
- HHAWQC based on that consumption rate, combined with other very conservative assumptions that are included in the HHAWQC calculation, ensure that risks of consuming fish from a single regulated waterbody are likely to be substantially overestimated and, therefore, will also be protective of individuals who are at the high end of the consumption distribution.

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APPENDIX B

A BRIEF REVIEW OF ISSUES RELEVANT TO THE ACCUMULATION OF PERSISTENT, BIOACCUMULATIVE, AND TOXIC (PBT) CHEMICALS BY SALMON

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1.0 INTRODUCTION

In September 2011 Washington State Department of Ecology (WDOE) issued Publication No. 11-09-050, *Fish Consumption Rates Technical Support Document, A Review of Data and Information about Fish Consumption in Washington*. This technical support document (TSD) was generated to support decision making regarding how to obtain an appropriate fish consumption rate (FCR) for use in calculating water quality standards for protecting human health (HHWQS). One of the issues WDOE raised in this TSD was whether consumption of salmon should be included in whatever FCR is ultimately used in these calculations, and if it is concluded that salmon should be included in an FCR, how to do so.

The driver behind this is human exposure to toxic chemicals, specifically via consumption of fish (or aquatic tissue in general). The greatest risk to human health from consumption of fish is generally understood to result from the presence of persistent, bioaccumulative, and toxic (PBT) chemicals. Thus the primary factor in determining the appropriateness of including consumption of salmon in an FCR is where salmon actually pick up these contaminants. A brief review of what is known about this subject is presented herein.

2.0 WHERE SALMON ACCUMULATE PBT CHEMICALS

As discussed by NOAA (2005), different runs of salmon exhibit different life histories. More specifically, NOAA described stream-type and ocean-type life histories. Behavioral attributes of these two general types of salmon are summarized in Table B1.

From Table B1, different species of salmon and different runs of the same species can exhibit distinctly different life histories, including how much time is spent in freshwater and where in freshwater systems this time is spent. These differences are potentially significant in that they may lead to differences in the mass (burden) of chemical contaminants (e.g., PBT chemicals) ultimately accumulated by the salmon, and in the fraction of this ultimate burden accumulated in freshwater vs. saltwater. Although the latter may not be relevant when assessing the risk to human health resulting from eating contaminated fish in general, it is relevant when considering what fraction of this overall risk results from accumulation of contaminants in freshwater systems vs. saltwater systems.

This last point is directly relevant to the question of whether there is any utility in including consumption of salmon in an FCR that will be used to drive remedial action(s) on the geographically limited scale of a single state. If a significant fraction of the contaminant burden found in salmon is accumulated in true freshwater systems it makes sense that the consumption of salmon be included in an FCR. However, if accumulation in the open ocean dominates, inclusion of salmon in an FCR makes no sense because there is no action the state can take that will have a significant effect on the contaminant burden found in returning adult salmon.

Table B1 A Summary of the Juvenile Characteristics of Stream and Ocean Life History Types

Stream-Type Fish	Ocean-Type Fish
Species	
Coho salmon	Coho salmon
Some Chinook populations	Some Chinook populations
Steelhead	Chum
Sockeye	Pink
Attributes	
Long period of freshwater rearing (>1 yr)	Short period of freshwater rearing
Shorter ocean residence	Longer ocean residence
Short period of estuarine residence	Longer period of estuarine residence
Larger size at time of estuarine entry	Smaller size at time of estuarine entry
Mostly use deeper, main channel estuarine habitats	Mostly use shallow water estuarine habitats, especially vegetated ones

[SOURCE: NOAA 2005]

Exclusion of salmon from an FCR does not imply that human exposure to contaminants due to consumption of salmon should not be accounted for when assessing overall risks to human health. Instead, these issues should be weighed when deciding whether salmon are accounted for when assessing the risks resulting from consumption of freshwater fish (by including consumption of salmon in an FCR) or when assessing the risks resulting from consumption of saltwater or marine fish (salmon would be backed out of the risk assessment for deriving a freshwater HHWQS via the relative source contribution or RSC). Ultimately, the issue of where the risks from consumption of salmon are counted appears to be an academic question. The more important factor (from the perspective of characterizing risk) is to ensure that consumption of salmon is not double counted by including it in both an FCR and as a component of the RSC.

In any case, the issue of salmon (or anadromous fish in general) is unique in that it is quite likely that a generic salmon will accumulate contaminants in both freshwater and saltwater habitats, and that the relative fraction accumulated in one habitat vs. the other will vary with species, run, and even individual. Taken to the extreme, this implies that each run needs to be evaluated independently to determine where contaminants are accumulated. However, much of the scientific literature supports accumulation in the open ocean as the dominant pathway for uptake of PBT chemicals by salmon, with the work of O'Neill, West, and Hoeman (1998), West and O'Neill (2007), and O'Neill and West (2009) providing perhaps the most thorough examination of the issue.

Figure B1 is taken from O'Neill and West (2009) and shows that levels of polychlorinated biphenyls (PCBs) in adult Chinook salmon (fillets) collected from a wide range of geographic locations are relatively uniform except for fish taken from Puget Sound, which show three to five times higher

levels of PCBs than fish taken from other locations. As discussed by the authors, these data can be interpreted as indicating accumulation of PCBs in Puget Sound and/or along the migratory routes of these fish, which, depending on the specific runs, can pass through some highly contaminated Superfund sites (e.g., Duwamish Waterway). However, O'Neill and West (2009) concluded that, on average, >96% of the total body burden (mass) of PCBs in these Puget Sound Chinook was accumulated in the Sound and not in natal river(s).

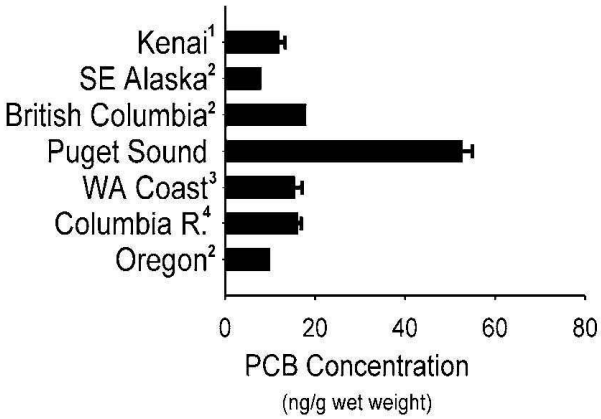

Figure B1 Average (±SE) PCB Concentration in Chinook Salmon Fillets
Data for Puget Sound were based on 204 samples collected by the Washington Department of Fish and Wildlife from 1992 to 1996; data for other locations were taken from the following (indicated by superscript numbers): [1]Rice and Moles (2006), [2]Hites et al. (2004; estimated from publication), [3]Missildine et al. (2005), and [4]United States Environmental Protection Agency (USEPA 2002)
[SOURCE: O'Neill and West 2009]

The basis for this conclusion is presented in Table B2, which compares PCB concentrations and body burdens in out migrating Chinook smolts collected from the Duwamish River and adults returning to the Duwamish.

Table B2 Concentration of PCBs (ng/g) and Body Burden of PCBs (total ng/fish) in Out-migrating Chinook Salmon Smolts and Returning Adults from the Contaminated Duwamish River, Washington

Variable	Smolts	Adults
Number of samples	80	34
Mean fish weight (g)	10	6,000
Whole body PCB concentration (ng/g)[a]		
Mean	170	57
95th percentile	860	88
PCB body burden (ng/fish)[a]		
Mean	2,100	350,000
95th percentile	9,200	800,000
Mean % of PCB body burden from the most contaminated smolts[b]	—	3.8

[a] Values for smolts are from J. P. Meador (National Oceanic and Atmospheric Administration Fisheries, Northwest Fisheries Science Center, personal communication); values for adults were estimated from measured muscle tissue concentration using the fillet–whole-body regression (see Methods) for PCBs.

[b] Contaminant data were only available for out-migrating subyearling smolts, so only samples with adults that went to sea as subyearlings were included in the analysis.

[SOURCE: O'Neill and West 2009]

These data show that even the most contaminated out migrating smolts contained no more than 4% of the body burden (mass) of PCBs found in returning adults. Thus, >96% of the PCB mass (burden) found in the returning adults was accumulated in Puget Sound. Even allowing for an order of magnitude underestimate in the body burden of out migrating smolts, O'Neill and West (2009) concluded that accumulation in freshwater would account for <10% of the average PCB burden ultimately found in adults returning to the Duwamish. By extension, this analysis supports the conclusion that Chinook salmon passing through uncontaminated estuaries during out migration accumulate a dominant fraction of their ultimate PCB body burdens in the open ocean. Other researchers have also reached this conclusion using their own data (e.g., Johnson et al. 2007; Cullon et al. 2009).

However, this analysis does not explain why Chinook salmon collected in Puget Sound exhibit higher concentrations of PCBs than Chinook salmon collected from other locations (Figure B1). Ultimately, O'Neill and West (2009) attributed this to a combination of factors, specifically PCB contamination of the Puget Sound food web (e.g., West, O'Neill, and Ylitalo 2008) combined with a high percentage of Chinook displaying resident behavior. That is, a large fraction of out migrating Chinook smolts take up permanent residence in the Sound, where they feed from a more contaminated food web than found in the open ocean. These factors would not affect Chinook runs or runs of any other species associated with natal rivers that discharge to saltwater outside Puget Sound.

Overall, these data support the position that, as a general rule, the predominant fraction of the ultimate PCB burden found in harvested adult fish is accumulated while in the ocean-phase of their life cycle (e.g., Cullon et al. 2009; Johnson et al. 2007; O'Neill and West 2009). Although this conclusion is specific to PCBs, there is no reason to suppose that it would not also hold for other legacy PBTs (e.g., DDT, dioxins) or globally ubiquitous PBTs (e.g., PBDEs, methylmercury) in general (e.g., Cullon et al. 2009). Because concerns about human consumption of fish are driven by risks from exposure to PBTs, driving the FCR higher by including salmon would thus appear to be of limited utility from the

perspective of protecting human health simply because these contaminants are accumulated in the ocean.

With that said, there are sufficient data to conclude that the food web in Puget Sound is contaminated with PCBs to a greater degree than the food web in the open ocean. To the extent that this is a result of true local sources (e.g., sediment hotspots), there may in fact be some "local" action that can be taken to reduce PCBs, or potentially other PBTs, in Puget Sound salmon. However, this is totally dependent on identification of localized sources amenable to remediation, and not simply a conclusion that the food web is contaminated (e.g., West and O'Neill 2007).

Again, simply increasing the FCR by including salmon will have essentially no positive effect on human health given that the dominant fraction of PBT body burdens in salmon appears to be accumulated in the open ocean, and not in waters immediately subject to in-state loadings.

3.0 PBT ACCUMULATION BY DIFFERENT SALMON SPECIES

As discussed, there is ample evidence that the body burdens of PBTs found in returning adult Chinook salmon depend to a significant extent on the life history of the specific run. Beyond this, there are interspecies differences in migratory and feeding behavior that suggest Coho, sockeye, pink, and chum salmon will not accumulate PBTs to the same extent as Chinook salmon under similar exposure scenarios (Groot and Margolis 1991; Higgs et al. 1995). Perhaps the most significant factor differentiating Chinook from the other salmon species is that Chinook tend to eat more fish (Higgs et al. 1995). Thus they effectively feed at a higher trophic level than the other species of salmon, and would be expected to accumulate greater burdens of PBT chemicals even when sharing the same habitat. This is in fact observable. For example, when looking at adult Chinook and Coho returning to the same rivers, O'Neill, West, and Hoeman (1998) found that Chinook muscle contained, on average, almost twice the total PCB concentrations found in Coho muscle. This was also true for adults collected in Puget Sound proper (O'Neill, West, and Hoeman 1998).

Differences between species can also manifest in sub-adults. For example, Johnson et al. (2007) reported ΣPCB concentrations in juvenile wild Coho collected from five different estuaries ranging from 5.9 to 27 ng/g (wet weight; whole body minus stomach contents). The corresponding range for wild Chinook juveniles collected from the same estuaries was 11 to 46 ng/g (wet weight; whole body minus stomach contents). Overall, PCB concentrations in juvenile Coho were, on average, equivalent to nominally 50% of those found in the paired Chinook juveniles. This is essentially the same ratio observed by O'Neill, West, and Hoeman (1998) in adult fish.

All this indicates that PBT residues in salmon will vary within species depending on the specific run, and between species regardless (i.e., even when different species share the same general habitat). Thus, grouping all salmon together does not provide an accurate assessment of PBT doses delivered to human consumers due to consumption of salmon. This suggests that human health risk assessments should, as a general rule, incorporate salmon on a species-specific basis, if not a run-specific basis.

Certainly, none of this is supportive of adopting a single default value for the dose of any contaminant received by humans via consumption of salmon. Thus adoption of a single default FCR for salmon is also not supported.

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APPENDIX C

FISH TISSUE CONCENTRATIONS ALLOWED BY USEPA AMBIENT WATER QUALITY CRITERIA (AWQC): A COMPARISON WITH OTHER REGULATORY MECHANISMS CONTROLLING CHEMICALS IN FISH

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1.0 INTRODUCTION

For chemicals that are capable of concentrating in fish, Ambient Water Quality Criteria for the Protection of Human Health (HH-WQC) are derived based on the uptake of the chemical by edible fish and an assumed level of fish consumption by anglers (USEPA 2000). It follows that for these chemicals, there is an allowable fish tissue concentration corresponding with each HH-WQC. The associated allowable concentrations are risk-based benchmarks analogous to other risk-based thresholds applied to edible fish in other circumstances and, therefore, the comparison with the more formal screening levels or guidelines is of interest. This appendix first describes how these allowable fish tissue concentrations, which are an integral component of the HH-WQCs, are derived. Next, several comparisons are presented between these allowable fish tissue concentrations and existing fish concentration data, concentrations found in other foods, as well as other guidelines or risk-based levels used for regulating chemical concentrations in edible fish, such as fish consumption advisory (FCA) "trigger levels" issued by state and federal agencies, and U.S. Food and Drug Administration (USFDA) tolerances, illustrating the differences in these values.

These comparisons will focus on a short list of chemicals for which an HH-WQC has been established and for which fish tissue concentration data are likely to be available. This list is comprised of the following chemicals:

- arsenic
- methyl bromide
- mercury (total, inorganic and organic)
- PCBs (total)
- chlordane; and
- bis-(2-ethylhexyl)phthalate (DEHP)

These six chemicals were selected based on several considerations: 1) propensity for accumulating in fish; 2) inclusion in fish tissue monitoring programs; 3) inclusion in recent studies measuring chemicals in other foods; 4) inclusion in specific analyses estimating human (dietary) intake; and 5) subject of FCAs in at least one state. Not all of these criteria were satisfied for each of the six example chemicals; nor did the available data allow comparisons to be made for all six chemicals; however, in general, at least four of the six chemicals could be included in each of the comparisons that were undertaken as part of this analysis.

2.0 ALLOWABLE FISH TISSUE CONCENTRATIONS DERIVED FROM THE HH-WQCS

The HH-WQCs are established based on two exposure pathways: use of surface water as a source of drinking water; and the consumption of fish that may be caught and eaten from the surface water. The

same algorithms that are used to calculate the HH-WQC can be rearranged to "back-calculate" an allowable fish tissue concentration.[11] Such values could be termed a water quality-based fish tissue concentration (FTC_{WQ}). These values are therefore a function of the same exposure assumptions, toxicity values and target risk level of 1×10^{-6} (for carcinogenic effects) used in calculating the HH-WQC.

The fish consumption rate (FCR) is an important factor in determining the HH-WQCs for chemicals having a moderate or high bioaccumulation potential. This analysis employs three different FCRs. As intended for the general population of fish consumers, we used the U.S. Environmental Protection Agency's (USEPA's) previously recommended default FCR of 6.5 grams/day or the current USEPA-recommended FCR of 17.5 grams/day. The choice between these two FCRs for each of the six chemicals was based on the derivation of the current HH-WQC, as published by USEPA. Specifically, the FCR used by USEPA to derive the current WQC for each chemical was selected for this analysis. For all but one chemical, this FCR was 17.5 grams/day. The exception was arsenic, where the HH-WQC is still based on an FCR of 6.5 grams/day. (The FTCs based on a FCR of 17.5 grams/day are referred to as the $FTC_{WQ\text{-}17.5}$ in the remainder of this appendix. Note that the recreational consumption rate FTC for arsenic is also referred to as $FTC_{WQ\text{-}17.5}$ despite being based on a FCR of 6.5 grams/day.)

Applying a FCR of 142.4 grams/day produced another set of FTC_{WQ} (referred to as the $FTC_{WQ\text{-}142}$ in this appendix); this FCR represents a higher-end fish intake, which USEPA specifically recommends for subsistence anglers and is similar to the FCR recently adopted by the state of Oregon for state-wide ambient water quality criteria (Oregon DEQ 2011). The resulting FTC_{WQ} for the six chemicals represent concentrations a regulatory agency might use to restrict consumption of fish in areas where there was reason to believe that subsistence fishing was known to occur. FTC_{WQ} calculated for the six chemicals are summarized in Tables C1a (based on a FCR of 6.5 or 17.5 gram/day) and C1b (based on a FCR of 142 gram/day).

FTC_{WQ} were derived from both the "water + organism" and the "organism only" HH-WQC. The former assumes that a surface water body is used as a source of drinking water and a source of fish consumption. The latter assumes that a surface water body is used only for consumption of fish. The influence of the drinking water consumption pathway is minor, or negligible for chemicals with a high bioconcentration factor (BCF), such as polychlorinated biphenyls (PCBs) and chlordane; however, it is important for chemicals with lower BCFs, such as methyl bromide, arsenic, and BEHP. For these chemicals, the use of the water and organism HH-WQC means that the allowable fish tissue concentration (i.e., FTC_{WQ}) will be substantially lower, because the target risk levels must be split between these pathways. However, the resulting FTC_{WQ} would be assumed to be applicable in most areas because most states require that surface water bodies be protected for use as a source of drinking water.

[11] Mathematically, this is the equivalent of multiplying the HH-WQC by the BCF, as long as a pathway-specific HH-WQC is used, i.e., based on the "organism only" or "water+organism" HH-WQC values.

Table C1a Allowable Fish Tissue Concentrations Derived from HH-WQC ($FTC_{WQ-17.5}$) for Six Chemicals: FCR = 17.5 g/day[1]

		HH-WQC Category[2]			
		Water+Organism		Organism Only	
Chemical	BCF (L/kg)	HH-WQC (µg/L, ppb)	$FTC_{WQ-17.5}$ (µg/kg, ppb)	HH-WQC (µg/L, ppb)	$FTC_{WQ-17.5}$ (µg/kg, ppb)
PCBs	31,200	6.4E-05	2.0	6.4E-05	2.0
Methyl bromide	3.75	47	178	1,493	5,600
Arsenic	44	0.018	0.77(1)	0.14	6.2
Mercury	7,343	0.054	394(3)	0.054	400
Chlordane	14,100	8.0E-04	11.3	8.1E-04	11.4
BEHP	130	1.2	15	2.2	286

Notes:
[1] Tissue concentration for arsenic was calculated based on former FCR of 6.5 g/day, because current HH-WQC still uses this value.
[2] Assumed use of the surface water body
[3] USEPA has established a Fish Tissue WQC for methylmercury of 300 ppb, which would be expected to supersede this value.

Despite the limited applicability of "organism only" FTC_{WQ} concentrations, they are still presented in some of the comparisons below because some regulatory agencies have derived FCA trigger levels based on fish consumption only or such triggers may be applied to waters not designated as a drinking water source (e.g., estuaries).

Table C1b Allowable Fish Tissue Concentrations Derived from HH-WQC (FTC_{WQ-142}) for Six Chemicals: FCR = 142 g/day

		HH-WQC Category[1]			
		Water+Organism		Organism Only	
Chemical	BCF (L/kg)	HH-WQC (µg/L, ppb)	FTC_{WQ-142} (µg/kg, ppb)	HH-WQC (µg/L, ppb)	FTC_{WQ-142} (µg/kg, ppb)
PCBs	31,200	7.9E-6	0.25	7.9E-6	0.25
Methyl bromide	3.75	38.7	145	184	690
Arsenic	44	4.9E-3	0.21	6.4E-3	0.28
Mercury	7,343	6.7E-3	49.2(2)	6.7E-3	49.3(2)
Chlordane	14,100	1.0E-04	1.4	1.0E-04	1.4
BEHP	130	0.24	31.8	0.27	35.2

Notes:
[1] Assumed use of the surface water body
[2] USEPA has established a Fish Tissue WQC for methylmercury of 300 ppb; this value does not apply to subsistence levels of fish consumption, but the unique approach applied to mercury by USEPA could have an effect on these values.

3.0 MEASURED FISH TISSUE CONCENTRATIONS IN U.S. LAKES AND RESERVOIRS: COMPARISON WITH FTC_{WQ}

Several federal and state programs have provided data on the fish tissue concentrations of environmental chemicals in U.S. lakes and rivers. In addition to nationwide programs sponsored by USEPA, such as the National Study of Chemical Residues in Fish (USEPA 1992), some states have ongoing fish monitoring programs or have sponsored targeted studies. Many of these programs are focused on a particular set of compounds or a particular area.

The National Study of Chemical Residues in Lake Fish Tissue (or "National Lake Fish Tissue Study", or NLFTS) was a statistically-based study conducted by USEPA Office of Water, with an objective of assessing mean levels of selected bioaccumulative chemicals in fish on a national scale. The results represent concentrations throughout the U.S. based on samples collected from 500 lakes and reservoirs in 48 states (USEPA 2009; Stahl et al. 2009). The sampling phase was carried out from late 1999 through 2003. The focus on lakes and reservoirs, rather than rivers and streams, was based on the greater tendency of lakes for receiving and accumulating environmental chemicals. A *National Rivers and Streams Assessment*[12] is currently in progress, and it would be of interest to examine the fish tissue concentration data from this survey when the data become available. It is likely that any fresh water survey of a national scope, whether it included bound or flowing water bodies would find a broad range of fish tissue concentrations, with the concentrations being more highly influenced by the location and history of the water body.

The NLFTS included PCBs, dioxins, polycyclic aromatic hydrocarbons (PAHs), 46 pesticides, arsenic and mercury. Adult fish were collected from two categories: predator and bottom-dwelling, with the predatory fish comprised of largemouth bass (50%), walleye (10%) and northern pike (7%), and bottom-dwelling species comprised of common carp (26%), white sucker (20%) and channel catfish (16%). A summary of the results from this study is shown in Table C2a.

Table C2a Concentrations in Fish as Reported by the National Lake Fish Tissue Study (USEPA 2009)

	Predator (Fillets) (µg/kg, ppb)			FTC_{WQ} Water+Organism (µg/kg, ppb)	
Chemical	Mean	50^{th} %ile	90^{th} %ile	$FTC_{WQ\text{-}17.5}$	$FTC_{WQ\text{-}142}$
PCBs	13.2	2.2	18.2	2.0	0.25
Arsenic	ND[(2)]	ND[(2)]	ND[(2)]	0.77	0.21
Mercury	352	285	562	394	49
Chlordane	ND[(2)]	ND[(2)]	3.6	11.3	1.4

Notes:

[1] National Lake Fish Tissue Study (NLFTS) (USEPA 2009); data from 486 predator fillet samples

[2] Infrequent detection in fish. Arsenic was detected at <1% of sampling locations, for predatory fish with a detection limit of 30 ppb. Chlordane was detected at 1-5% of sampling locations (for predatory fish) with a detection limits of 0.02 (alpha) and 0.49 (gamma) ppb. BEHP was detected at 1-5% of sampling locations (for predatory fish) and results are not provided by USEPA (2009).

[12] http://water.epa.gov/type/rsl/monitoring/riverssurvey/index.cfm

The NLFTS was not focused on areas specifically affected by industrial activities or historic releases. The water bodies included in this survey were selected at random with an objective of capturing typical levels of the chemicals analyzed. In fact, many lakes were included that could be regarded as pristine, likely to have been affected by only minimal human activity. Therefore, the resulting data could be representative of 'background' concentrations, which are from unavoidable depositional inputs of the chemicals of interest. However, because many of the water bodies included the NLFTS may have been affected by specific discharges or historic releases, we refer to the resulting data being only representative of typical levels for U.S. lakes. For simplicity, only the data representing predatory fish were included in this analysis, because these are the species likely to be targeted by anglers. The bottom-dwelling fish, which were included in the NLFTS to represent ecological (wildlife) exposures, contained substantially higher concentrations of PCBs (6 times greater at the median) and chlordane (1.7 ppb vs. ND), but lower concentrations of mercury (4 times lower at the median).

As shown in Table C2a, this study provided data for PCBs and mercury, as well as for arsenic and chlordane. Arsenic and chlordane were reported at very low frequencies of detection making quantitative comparisons between fish concentrations and FTCs challenging. Nevertheless, because the detection limits for chlordane (0.02 ppb for alpha and 0.5 ppb for gama) are less than the $FTC_{WQ-17.5}$ (11.3 ppb), and the 90th percentile of the distribution of chlordane concentrations is roughly 3 times lower than the $FTC_{WQ-17.5}$, NLFTS data do demonstrate that chlordane concentrations in predatory fish from the large majority of U.S. surface waters are below the $FTC_{WQ-17.5}$. This also suggests that current concentrations of chlordane in most U.S. surface waters are unlikely to be above the HH-WQC derived based on the consumption rate of recreational anglers.

A similar evaluation could not be conducted for arsenic. The reported arsenic detection limits was above the $FTC_{WQ-17.5}$ derived from the HH-WQC, precluding a comparison with the $FTC_{WQ-17.5}$ absent making assumptions about the concentration of arsenic in fish samples with non-detectable concentrations. As a specific example, the NLFTS reported a method detection limit (MDL) for inorganic arsenic of 30 ppb, even using a state-of-the-art analysis, Method 1632A for the speciation of arsenic. Given that the $FTC_{WQ-17.5}$ for arsenic is 0.77 ppb, it is not possible to determine whether concentrations in predator fillets are above or below that $FTC_{WQ.}$ Assuming detection limits for arsenic cannot be easily refined, this comparison does suggest that it is not possible to demonstrate compliance with the arsenic $FTC_{WQ-17.5.}$

For PCBs, the NLFTS data indicate that a substantial portion of predatory fish from U.S. lakes exceed the $FTC_{WQ-17.5}$ for PCBs (2 ppb). The extent of this exceedance depends on whether the data are represented by the mean concentration (13.2 ppb), which exceeds the $FTC_{WQ-17.5}$ by a factor of about 6x, or the median (i.e., 50th percentile) concentration (2.3 ppb), which is nearly equivalent to the $FTC_{WQ-17.5}$. While this comparison indicates the average concentration of PCBs in fish throughout the U.S. is substantially higher than the $FTC_{WQ-17.5}$, it does not follow that fish in most surface waters of the U.S. have PCB concentrations greater than both of the FTC_{WQ}s. The difference between the mean and median concentration comparisons for this data set likely arises because the data are skewed, with the majority of samples having relatively low concentrations. As noted above, the 50th percentile of the distribution of PCB concentrations in predatory fish from U.S. lakes is approximately equal to the $FTC_{WQ-17.5}$. Assuming the BCF accurately reflects the relationship between the PCB concentration in fish and water, the comparison of the $FTC_{WQ-17.5}$ to the 50th percentile indicates that roughly half of sampled U.S. waters had PCB concentrations that met or were below the HH-WQC derived based on the consumption of recreational anglers. .

The mean mercury concentration of the NLFTS data (352 ppb) is slightly lower than the $FTC_{WQ-17.5}$ for mercury (394 ppb). The percentile data provided by USEPA (2009) indicate the distribution of

mercury concentrations in predatory fish is also skewed, though a smaller proportion of the samples (approximately 25%) exceed the mercury $FTC_{WQ-17.5}$ than exceeded the PCB $FTC_{WQ-17.5.}$

The results of parallel comparisons with FTCs derived based on subsistence anglers (i.e., FTC_{WQ-142}) lead to a different conclusion for three for the four compounds (chlordane, PCBs and mercury). The arsenic FTC_{WQ-142} is about four times lower than the $FTC_{WQ-17.5}$ and is also below the typical detection limits for inorganic arsenic, precluding any meaningful quantitative comparisons with the FTC_{WQ-142}.

The detection limit for alpha chlordane is slightly above the FTC_{WQ-142} and the detection limit for gamma is slightly below (see footnotes to Table C2a). Additionally, the 90th percentile of the distribution of chlordane concentrations is only about 2.5 times higher than the $FTC_{WQ-142.}$ These comparisons suggest that typical concentrations of chlordane may be similar to or less than the FTC_{WQ-142} in many U.S. surface waters, though the upper percentiles of the distribution do exceed the FTC_{WQ-142}, in some cases, substantially (Table C2a).

The FTC_{WQ-142} is about 10 times lower than the $FTC_{WQ-17.5}$ for PCBs and mercury (Table C2a). With the increase in FCR, the average fish tissue concentration exceeds the FTC_{WQ-142} by approximately 50x and 7x for PCBs and mercury, respectively (Table C2a). Additionally, the majority of the distribution of PCB and mercury concentrations is above the $FTC_{WQ-142.}$ For both chemicals, the concentration at the 5th percentile of the distribution exceeds the $FTC_{WQ-142.}$ These comparisons indicate that if HH-WQC were to be revised using an FCR of 142 grams/day, assumed to be representative of subsistence anglers, the concentrations of PCBs and mercury in fish from virtually all surface waters in the U.S. would exceed the allowable fish concentration associated with such an HH-WQC.

Several state programs have surveyed fish tissue concentrations, often including PCBs, metals and/or pesticides. The state data assembled for our analyses included surveys conducted by Washington State Department of Ecology (WA-DOE) and by the Florida St. Johns River Water Management District (SJRWMD). Overall, the state programs include more recent data (through 2011) than those presented in the NLFTS (through 2003). These are much more limited data sets compared to the data from the NLFTS. Additionally, the number of observations from each state varies by chemical and in some instances all the data points are from a single state (e.g., all PCB data are from Washington).

Table C2b Measured Concentrations in Fish Samples from Washington and Florida

	Data from State Programs (µg/kg, ppb)			FTC_{WQ}[1] (µg/kg, ppb)	
Chemical	Mean[2]	50th %ile	90th %ile	$FTC_{WQ-17.5}$	FTC_{WQ-142}
PCBs	27.4	22.1	49.8	2.0	0.25
Mercury	191	120	408	394	49
Chlordane	1.4	0.62	2.8	11.3	1.4

Notes:
Based on data provided by J. Beebe (NCASI) and comprised of data from Washington State WA-DOE (2011), WA-EIMS, http://www.ecy.wa.gov/eim), and St. Johns River Water Management District (SJRWMD), Florida (http://sjr.state.fl.us).
[1] FTC_{WQ} derived from water and organism HH-WQC.
[2] Data included: for PCBs, 45 samples from WA-EIMS; for mercury, 1598 samples from WA-EIMS and SJRWMD; and for chlordane, 382 samples from SJRWMD.

The mean concentration of PCBs in predatory fish (27.4 ppb), is about 14 times and 100 times higher than the $FTC_{WQ-17.5}$ and FTC_{WQ-142}, respectively. In fact, both FTC_{WQ}s are well below the minimum reported concentration (9.7 ppb) from this data set. Assuming these data were collected from waters potentially affected by PCB releases suggests that meeting the HH-WQC, based on either the recreational of subsistence FCR, in such waters is likely to be a challenge. To the extent these data are only from Washington, this finding may only apply to waters of that state.

The mean concentrations of mercury and chlordane from state programs are below their respective $FTC_{WQ-17.5}$ by approximately 2x- and 8x-, respectively (Table 4-2b) suggesting that a substantial portion of the surface waters in these states would meet an HH-WQC derived based on an FCR assumed to be representative of a recreational angler. The mean concentration of chlordane is equal to the FTC_{WQ-142}. If the chlordane distribution from these two states has a similar "shape" to the distribution in the national survey, this comparison suggests that a substantial portion of surface waters in these two states would meet an HH-WQC based on an FCR representative of a subsistence angler. Fewer waters are likely to meet such an HH-WQC for mercury, given that the mean concentration exceeds the FTC_{WQ-142} by approximately 4x.

Arsenic was included in several of the state databases, however, inorganic arsenic was not detected at measurable concentrations. As discussed above for the NLFTS data, meaningful comparison of inorganic arsenic concentrations to FTCs is precluded because MDLs are greater than the FTCs.

4.0 COMPARISON OF FTC_{WQ} TO FCA TRIGGER LEVELS ESTABLISHED BY STATE OR OTHER PUBLIC HEALTH AGENCIES

Most states and various federal agencies have programs for the protection of anglers who may eat fish containing trace amounts of chemicals. These programs are responsible for issuing FCAs for lakes and reservoirs where particular chemicals have been detected at levels in fish that exceed some risk-based "trigger level." While the approach to setting FCAs may differ, most programs use a risk-based approach to develop guidelines that are intended to be protective of the health of the angler communities with a wide margin of safety. USEPA (2000) issued guidance that could be used to establish some uniformity in the methods used to derive FCAs, but most states are maintaining programs and guidelines that have served them for many years. A common feature of both federal and state guidelines is the movement away from a single trigger level and towards a progression of trigger levels, each associated with an increasing level of restricted intake for the fish (and chemical) in question. Despite this increased complexity, USEPA (2000) also provided screening values (SV) based on moderate (recreational) and high (subsistence) levels of fish consumption, termed SVrec and SVsub, respectively, and shown in Table 4-3 for PCBs, arsenic, chlordane, and mercury.

Also shown in Table 4-3 are examples of FCA trigger levels from state programs that publish numerical benchmarks for this purpose. For states that have adopted a series of trigger levels, this analysis presents the levels based on either a "no more than 2 meal per month" restriction (noted as "L2" in Table 4-3), or a 'do not eat' advisory (complete restriction, notes as "R" in Table 4-3). Two 8-ounce (227 g) meals per month is assumed to be comparable to the 17.5 gram/day FCR applied by USEPA to the derivation of HH-WQC.[13]

[13] The guidelines from WI-DNR and MI-DCH, however, only included a one meal per month advisory level, and the concentrations accompanying this advisory level are shown for these two agencies (noted as "L1" in Table 4-3).

Table C3 USEPA Screening Values for Fish and FCA Trigger Levels Used by Select State Agencies[1]

	Federal USEPA (2000)[2] (µg/kg, ppb)		Select State Programs (µg/kg, ppb)			FTC_{WQ} Organism Only Values (µg/kg, ppb)	
Chemical	SV(rec)[3]	SV(sub)[3]	WI-DNR	MI-DCH	WV-DHHS	$FTC_{WQ\text{-}17.5}$	$FTC_{WQ\text{-}142}$
PCBs	20	2.5	220 (L1) 2,000 (R)	200 (L1) 2,000 (R)	150 (L2) 1,340 (R)	2.0	0.25
Arsenic	26	3.3	--	NA	140 (L2) 1,250 (R)	6.2	0.28
Mercury	400	50	500-1000 (NS)	500 (L) 1,500 (R)	220 (L2) 1,880 (R)	400	49
Chlordane	114	14	660 (L1) 5,620 (R)	300 (NS)	880 (L2) 7,660 (R)	2.2	1.4

Notes:
R: Restricted, referring to 'do not eat' advisory.
L: Limited, or a limited amount of consumption is advised.
L1: Limited to 1 meal per month.
L2: Limited to 2 meals per month.
NS: Not stated whether the value represents a restriction or a limit.
[1] Wisconsin Department of Natural Resources (WI-DNR), 2007, 2011; Michigan Department of Community Health (MI-DCH), 2008; West Virginia Department of Health and Human Services (WV-DHHS).
[2] USEPA, 2000. Guidance for Assessing Chemical Contaminant Data for Use in Fish Advisories, Volume 1.
[3] Screening values (SV) for the recreational and subsistence angler.

When compared to these FCA trigger levels, the $FTC_{WQ\text{-}17.5}$ for PCBs, arsenic and chlordane are 20-4,000 times lower (more stringent) (Table C3). For mercury, the $FTC_{WQ\text{-}17.5}$ is comparable to the trigger levels prompting some restriction on fish consumption, but is as much as 4x lower than the level where a 'do not eat' advisory is prompted. $FTC_{WQ\text{-}142}$ are between 200-8,000 times lower than the FCA trigger levels for PCBs, arsenic, and chlordane, and 4 to 40 times lower than the trigger levels for mercury (Table C3).

As shown in Table C3, the USEPA SVs are either similar or 10x higher than the FTC_{WQ} derived from the HH-WQC. Because these USEPA values are intended to be generic screening-level benchmarks, they are very conservative compared to the trigger levels used by the most state programs (discussed further below).

Comparing the USEPA SVs to FTC_{WQ} for chemicals for which noncancer endpoints are the driver, such as mercury, SVs are the same as the FTC_{WQ}s. For the other three constituents, for which the cancer endpoint is most sensitive, the SVs are approximately 10 times higher, because SVs are derived based on a $1x10^{-5}$ target risk level, rather than a $1x10^{-6}$ target risk level.

In contrast, fish advisory trigger levels used by public health agencies in Wisconsin, Michigan, and West Virginia (Table C3) are less stringent, and in general, would require substantially higher concentrations of arsenic, chlordane and PCBs than allowed by the HH-WQC before issuing even a moderate restriction on fish consumption. Based on our survey of state "trigger levels" and recent

reviews comparing the FCAs between states (IWG-ACA, 2008; Scherer et al. 2008), we believe that the FCAs from Wisconsin, Michigan, and West Virginia are likely to be representative of the FCAs from many state programs. Scherer et al. (2008) found the FCAs among states to be quite similar, despite some variation in the methods used to develop the FCAs. Many state programs rely on less-stringent food tolerance levels as the basis for their trigger levels; this choice is consistent with the desire by States to consider the value of their recreational fisheries and the benefits of fish consumption, while protecting the public from potential chemical risks. The difference in the State vs. EPA trigger levels is due to several factors. As noted previously, state guidelines are typically based on a series of FCA trigger levels, giving the States the ability to partially restrict fish consumption at many concentration levels. Further, the ability to issue consumption limits for specific target fish species also permits states to allow higher fish tissue concentrations. Lastly, state agencies are more likely to apply lower assumed fish consumption rates based on local or regional surveys conducted within the state.

A key illustration of the conservative nature of the FTCs is provided by a comparison of the proportion of samples in the NLFTS data set that exceed an FTC_{WQ} to the proportion of waters in the U.S. that have a fish consumption advisory. As described above approximately 50% of fish samples have PCB concentrations that exceed the $FTC_{WQ\text{-}17.5}$ and over 95% exceed the $FTC_{WQ\text{-}142}$. Yet, only about 15% of the nation's lakes are subject to a fish consumption advisory (USEPA 2009). Given that a goal of both an HH-WQC and an FCA is protection of the health of anglers, the much larger proportion of waters estimated to potentially pose an unacceptable risk when an HH-WQC is used than measured by the posting of an FCA, suggests that the derivation of HH-WQC by USEPA is substantially more conservative than the derivation of FCAs by state agencies.

5.0 COMPARISON OF FTC_{WQ}S TO HEALTH-BASED LIMITS FOR FISH OR OTHER FOODS

Other federal and global agencies charged with protection of food safety have established guidelines for ensuring the safety of foods in commerce. The most notable examples in the U.S. are the food tolerances established by USFDA. These tolerances have been used as a guideline for assessing the safety of food, largely animal products, such as beef, chicken, fish, milk and eggs. These tolerances are typically less stringent than analogous values derived using USEPA methods for risk assessment. Unlike the USEPA, the USFDA must balance potential economic concerns with the potential benefits to public health; in other words, the USFDA must consider the consequences of its actions on the U.S food supply. USEPA exposure limits and screening levels may also be considered for their economic consequences, but this review is conducted outside of the Agency and only after the value has been derived. Regardless, USFDA tolerances are risk-based concentrations and many risk assessors and scientists support the idea that the tolerances are protective of the public health (Cordle et al. 1982; Maxim and Harrington 1984; Boyer et al. 1991). Due to recent incidents in Europe in which PCBs were accidentally introduced into animal feeds, the European Commission (EC) has set maximum levels for PCBs in foods and feedstuffs, including fish (EC, 2011). The limits were based on a report of the European Food Safety Authority (EFSA) deriving allowable exposure levels, and on monitoring data compiled throughout the European Union (EU). The EU considered both the public health protection and the feasibility of attaining these limits, based on current levels measured in foods.

FTC_{WQ} derived from the HH-WQC are in all cases well below both the USFDA and EU food tolerance levels (Table C4). The USFDA tolerance for PCBs in fish of 2,000 ppb is 1,000 times higher than the $FTC_{WQ\text{-}17.5}$ and 8,000 times higher than the $FTC_{WQ\text{-}142}$.

Table C4 Comparison of FTC_{WQ} to Food Safety Guidelines for Chemical Concentrations in Fish

	Food Safety Standards		HH-WQC-Based Threshold for Fish	
Chemical	USFDA Tolerance for Fish[1] (µg/kg, ppb)	EU Limit for Fresh Fish[2] (µg/kg, ppb)	FTC_{WQ} FCR = 17.5 (µg/kg, ppb)	FTC_{WQ} FCR=142 (µg/kg, ppb)
PCBs	1,000 (action level) 2,000 (limit)	250[(3)]	2.0	0.25
Mercury	1,000 (action limit)	--	394	49.2
Chlordane	300	--	11.3	1.4

Notes:
[1] USFDA (1998, 2011); Values are based on wet weight.
[2] European Commission (EC) 2011. Commission Regulation No. 1259/2011.
[3] EC Limit for PCBs is 125 ng/g wet wt. for the sum of 6 'marker' congeners, which comprise about 50% of the PCBs in fish. Therefore, to be applicable to a measure of total PCBs, this value was multiplied by a factor of 2 (EC, 2011).

6.0 TYPICAL INTAKES OF THE CHEMICALS IN THE U.S. POPULATION: COMPARISON TO THE ALLOWABLE DAILY INTAKES DERIVED FROM THE HH-WQC

The goal of an HH-WQC is to limit exposure of the population to chemicals in water such that an allowable dose (or risk) is not exceeded. If the dominant exposure pathway for a chemical is direct contact or use of surface water, then compliance with the AWQC may, indeed, limit overall exposure to allowable levels. However, if other pathways also contribute to overall exposure and, in particular, if the other pathways represent larger exposures than surface water, then establishment and enforcement of a stringent surface water criterion may not provide a measurable public health benefit. This section compares exposures allowed by the HH-WQC to the potential exposures from a limited set of other exposure sources or pathways for five chemicals.

One of the key assumptions used to derive FTC_{WQ} is an allowable daily intake of each constituent in question. This allowable daily intake is a toxicologically-derived value and is represented by a reference dose (RfD) (for noncancer endpoints) or a risk-specific dose (RSD) (when cancer is the endpoint). The RSD is equal to the target risk level (typically 1×10^{-6}) divided by the cancer slope factor (CSF) for a particular constituent.

As shown in Table C5, the RfDs and RSDs for the six chemicals evaluated in this appendix range from 0.35 µg/day for PCBs to 98 µg/day for methyl bromide.[14] These are the toxicity values chosen by USEPA for the derivation of HH-WQC.

Another way to estimate the allowable daily dose associated with the HH-WQC, and the FTC_{WQ} in particular, is to multiply the allowable fish tissue concentrations (i.e., the FTC_{WQ}) by the assumed FCR of 17.5 grams/day. The results, as shown in Table C5 as "Fish Dose", represent the dose of each chemical that someone would receive who ate fish containing chemicals at concentrations equal to the FTC_{WQ}.

[14] Traditional units of dose in mg/kg-day are converted to units of intake (µg/day) by multiplying by an adult body weight of 70 kg and a conversion factor of 1000 µg/mg.

For PCBs, mercury and arsenic, very low, but measurable daily intakes by the U.S. population are based on releases of these substances into the environment and their presence in trace quantities in the food supply. Arsenic occurs naturally in soils and groundwater and, therefore, there is a normal daily intake that varies by region. For BEHP, the presence of trace amounts in food stems from its use in plastic food packaging materials (Fromme et al. 2007). A summary of the data used to provide an estimate of the typical daily intake of each chemical is presented below.

PCBs: The intake of PCBs through foods, mainly animal products, has declined dramatically in the last 30 years. However, Schecter et al. (2010) recently carried out a market-basket survey of several types of foods and found measurable levels in enough foods to propose a daily intake of about 0.1 µg/day for a typical resident of the U.S. Other studies in Europe have proposed slightly higher intake levels (as high as 0.8 µg/day), but overall, corroborate the findings of Schecter et al. (2010). This range of typical dietary intakes of PCBs is 3 times to as much as 20 times greater than the risk-specific dose (RSD) used to derive the HH-WQC (0.035 µg/day) (Table C5). Thus, the HH-WQC is based on an exposure limit for PCBs that is routinely exceeded by the typical PCB intake that occurs through dietary exposures.

BEHP: Considerable effort has been made to estimate the human exposure to phthalate esters, which arises from food packaging materials, e.g., plastic food wraps. A German study by Fromme et al. (2007) provides the most reliable estimates of intake, based on a study using both samples of dietary items and biomonitoring data. Because phthalate ester exposures are derived from plastic packaging/wrapping that is sold across the globe, intakes estimated by this study for a German population are likely to be comparable to those in U.S. The authors report a median BEHP intake of 2.4 µg/kg-day (162 µg/day) which is approximately 30 times greater than the RSD used by the HH-WQC (Table C5). Thus, the HH-WQC is based on an exposure limit for BEHP that is routinely exceeded by the typical intake that occurs through dietary exposures.

Table C5 Allowable vs. Actual Daily Intakes for Select Chemicals

	Allowable Daily Intakes Used as the Basis for the HH-WQCs		Measured or Estimated Average Daily Intakes Derived from Food		
	Value [RfD or RSD] (µg/day)	Fish Dose[1] (µg/day)	Intake (µg/day)	Group	Note
PCBs	0.035 [RSD]	0.035	0.1-0.8	all	(a)
Methyl bromide	98 [RfD]	3.1	6.5 (mean); 310 (95th %ile)	male	(b)
			10 (mean); 350 (95th %ile)	female	
Arsenic	0.04 [RSD]	0.014	3.6 / 2.7 (avg.); 9.4 (90th %ile)	male	(c)
			2.8 / 2.4 (avg.); 11.4 (90th %ile)	female	
Mercury	7 [RfD]	7	8.6 (mean); 166 (90th %ile)	male	(d)
			8.2 (avg.); 204 (90th %ile)	female	
BEHP	5 [RSD]	0.26	162 (median); 309 (95th %ile)	all	(e)

Notes:
RfD, Reference Dose; RSD, Risk-Specific Dose
[1] Computed as FTC_{WQ} [from Table C1a] x FCR [17.5 g/day]
(a) Range is based on the results of several studies (Darnerud et al. 2006; Arnich et al. 2009; Roosens et al. 2010; Schecter et al. 2010).
(b) Cal-EPA 2002; assumed body weight of 70 kg for adults.
(c) Meacher et al. 2002; assumed body weight of 70 kg for adults.
(d) MacIntosh et al. 1996.
(e) Fromme et al. 2007.

Arsenic: A study by Meacher et al. (2002) represents a comprehensive evaluation of total inorganic arsenic exposure in the U.S. population. The authors discuss other studies with a similar aim and conclude that the average daily intake, primarily from food and drinking water, is in the range of 1 to 10 µg/day. Estimates of average daily intakes are 60 to 90 times greater than the RSD. Thus, the HH-WQC is based on an exposure limit for arsenic that is exceeded by a wide margin, by typical dietary intakes of arsenic.

Methyl bromide: The concentrations detected in foods are mainly in animal products, such as milk, which makes estimates of a one-time exposure as high as 4-5 µg/kg-day, but with average daily exposures likely to be less than 1 µg/kg-day, according to a study by Cal-EPA (2002). While 95th percentile values (310-350 µg/day) are more than 40 times higher that the mean intake estimates, it can be concluded that typical methyl bromide intakes based on diet are likely to be below the RfD of 98 µg/day. Thus, for methyl bromide, dietary intakes would not appear to hinder the objective of limiting the exposures based on fish consumption.

Mercury: The predominant human intake is from concentrations in predatory and deep-sea fish such as tuna. Average daily intakes are estimated to be about 8 µg/day (MacIntosh et al. 1996) and are comparable to the RfD of 7 µg/day (Table C5). Thus, for mercury, it is not uncommon for the consumption of store-bought tuna to provide an intake equivalent to the RfD; achieving this level of exposure would at least appear to be an achievable public health objective.

In summary, estimated daily intakes for five of the six chemicals could be obtained from the literature (Table C5). For PCBs, arsenic and BEHP, the chemicals for which potential cancer risk is the most sensitive endpoint, the estimated daily intake for the U.S. population is between 3 times to 90 times greater than the RSD. In surface waters with fish that have concentrations that are no more than a 2-times lower than the FTC, based on the comparisons shown in Table C5, decreasing exposures to the levels associated with HH-WQC would be likely to have no discernible effect on the intake of these chemicals in the community.

7.0 SUMMARY AND CONCLUSIONS

This paper described the derivation of allowable fish tissue concentrations (referred to as FTC_{WQ}) associated with HH-WQC for a select group of chemicals. FTC_{WQ} are based on the same exposure and toxicity factors used to derive the HH-WQC. Separate FTC_{WQ} were derived for USEPA's recommended fish consumption rate for recreational anglers (17.5 grams/day, $FTC_{WQ\text{-}17.5}$) and subsistence anglers (142 grams/day, $FTC_{WQ\text{-}142}$). Given the nearly 10x higher consumption rate assumed for subsistence anglers compared to recreational anglers, $FTC_{WQ\text{-}142}$ were lower than the $FTC_{WQ\text{-}17.5}$ for every chemical by about 10x. FTC_{WQ} were compared to: (1) concentrations measured in fish from U.S. water bodies; (2) trigger levels used by State agencies to set fish consumption advisories; and (3) allowable concentrations set by other US and international health agencies. Additionally, ADIs used to derive FTC_{WQ} were compared to estimated daily dietary intakes from all sources.

PCB concentrations in about half of the fish from the NLFTS exceeded the $FTC_{WQ\text{-}17.5}$ and PCB concentrations in essentially all fish from the NLFTS exceeded the $FTC_{WQ\text{-}142}$. (Additionally, all of the fish from two state-specific surveys had PCB concentrations above the $FTC_{WQ\text{-}17.5}$ and the $FTC_{WQ\text{-}142}$.) The mercury concentrations for the majority of fish in the NLFTS were below the $FTC_{WQ\text{-}17.5}$ but most fish had mercury concentrations above the $FTC_{WQ\text{-}142.}$ Chlordane was not detected in the majority of NLFTS samples with detection limits below the $FTC_{WQ\text{-}17.5}$ and the $FTC_{WQ\text{-}142}$ suggesting the majority of fish have chlordane concentrations below either FTC_{WQ}. Arsenic was not detected in majority of NLFTS; however, unlike chlordane, the method detection limit for arsenic exceeds both the $FTC_{WQ\text{-}17.5}$ and the $FTC_{WQ\text{-}142}$ by more than 30x, precluding the possibility of determining whether arsenic concentrations meet the HH-WQC. Thus, whether nationwide fish tissue concentrations meet the FTC_{WQ} depends upon the chemical of interest and whether recreational or subsistence angler consumption rates are used to derive the $FTC_{WQ.}$ It does appear that if HH-WQC were to be revised using an FCR of 142 grams/day, the concentrations of PCBs and mercury in fish from virtually all surface waters in the U.S. would exceed the allowable fish concentration associated with such HH-WQC.

$FTC_{WQ\text{-}17.5}$ for PCBs, arsenic, and chlordane were 20 to 4,000 times lower (more stringent) than FCA trigger levels commonly used by state programs. For mercury, the $FTC_{WQ\text{-}17.5}$ was comparable to typical state trigger levels prompting some restriction on fish consumption, but it was as much as 4 times lower than the level where a 'do not eat' advisory is prompted. Again, the comparisons were much more remarkable using the $FTC_{WQ\text{-}142}$. $FTC_{WQ\text{-}142}$ were between 200 times and 8,000 times lower than the FCA trigger levels for PCBs, arsenic, and chlordane, and 4 times to 40 times lower than the state trigger levels for mercury. These comparisons were based on the guidelines from a select number of states, including Wisconsin, Michigan, and West Virginia; however, the FCA trigger

levels were comparable among this small group of states, and based on our review of guidelines in many other states not included in this analysis, we believe that these states can be considered representative of many other state programs.

A comparison of FCAs to the NLFTS data provides another comparison that highlights the conservatism of the FTC_{WQ} (and the HH-WQC from which they were derived). Approximately 50% of fish samples from the NLFTS had PCB concentrations that exceeded the $FTC_{WQ-17.5}$ and over 95% exceeded the FTC_{WQ-142}. However, only about 15% of the nation's lakes and reservoirs (on a surface area basis) are subject to a FCA based on PCBs (USEPA 2009). Thus, use of HH-WQC indicated that a much larger proportion of US surface waters pose an unacceptable risk than indicated by FCA postings. This comparison further illustrates that the assumptions used by USEPA to derive HH-WQC are more conservative than the assumptions used by state agencies to derive FCAs.

Various agencies, both Federal and international, have established concentration limits for fish as a food in commerce. The FDA food tolerances are the most notable example. FTC_{WQ} were compared to FDA tolerance limits and a recently established EU limit for PCBs in fish. The $FTC_{WQ-17.5}$ for PCBs of 2 ppb is 500 times lower than the FDA action limit of 1,000 ppb and 125 times lower than an EU limit of 250 ppb. The FTC_{WQ-142} is 1,000x and 4,000x lower than the EU and FDA action limits, respectively. The FDA tolerance of 300 ppb for chlordane is similarly much less stringent than either the $FTC_{WQ-17.5}$ (11.3 ppb) or the FTC_{WQ-142} (1.4 ppb) for chlordane. The FDA action level for mercury of 1,000 ppb is similar to but still higher than either the $FTC_{WQ-17.5}$ (394 ppb) or the FTC_{WQ-142} (49 ppb) for mercury. These comparisons indicate that HH-WQCs are limiting fish tissue concentrations to levels substantially below those considered to be without significant risk by public health agencies whose goal is to ensure the safety of edible fish.

Lastly, allowable daily intakes (RfDs for noncancer endpoints, RSDs for the cancer endpoint) assumed by the FTC_{WQ} were compared to estimates of the daily intake of arsenic, BEHP, mercury and PCBs obtained from the open literature. Specifically, daily intakes were taken from studies that measured concentrations in various foodstuffs. Typical daily dietary intakes of arsenic, BEHP and PCBs exceeded the allowable daily intakes used to derive HH-WQC by a substantial margin. The typical daily dietary intake of mercury, mostly from tuna, is comparable to the RfD used to derive the HH-WQC. Thus, for those compounds whose daily dietary intake is greater than the intake associated with surface water and already exceeds the allowable daily intakes used to establish HH-WQC, the establishment and enforcement of a more stringent HH-WQC may not provide a measurable public health benefit.

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ATTACHMENT I

Derivation of Human Health-Based Ambient Water Quality Criteria: A Consideration of Conservatism and Protectiveness Goals

Derivation of Human Health-Based Ambient Water Quality Criteria: A Consideration of Conservatism and Protectiveness Goals

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ABSTRACT

Under the terms of the Clean Water Act, criteria for the protection of human health (Human Health Ambient Water Quality Criteria [HHWQC]) are traditionally derived using US Environmental Protection Agency (USEPA) recommended equations that include parameters for exposure assessment. To derive "adequately protective" HHWQC, USEPA proposes the use of default values for these parameters that are a combination of medians, means, and percentile estimates targeting the high end (90th percentile) of the general population. However, in practice, in nearly all cases, USEPA's recommended default assumptions represent upper percentiles. This article considers the adequacy of the exposure assessment component of USEPA recommended equations to yield criteria that are consistent with corresponding health protection targets established in USEPA recommendations or state policies, and concludes that conservative selections for exposure parameters can result in criteria that are substantially more protective than the health protection goals for HHWQC recommended by USEPA, due in large part to the compounding effect that occurs when multiple conservative factors are combined. This situation may be mitigated by thoughtful selection of exposure parameter values when using a deterministic approach, or by using a probabilistic approach based on data distributions for many of these parameters. *Integr Environ Assess Manag* 2014;9999: XX--XX. © 2014 SETAC

Keywords: Conservatism Human health Water quality criteria

INTRODUCTION

Section 304(a)(1) of the Clean Water Act (CWA) requires the US Environmental Protection Agency (USEPA) to develop and publish recommended numeric ambient water quality criteria (AWQC) for limiting the impact of pollutants on human health and aquatic life. These recommended human health-based ambient water quality criteria (HHWQC) are intended to provide guidance for states and tribes to use in adopting their own water quality standards and are meant to "minimize the risk of adverse effects occurring to humans from chronic (lifetime) exposures to substances through the ingestion of drinking water and consumption of fish obtained from surface waters" (USEPA 2000a).

During the course of recent regular reviews of water quality criteria, a number of states have received stakeholder opinions, via public meetings or during open comment periods, suggesting that certain water quality criteria may be insufficiently protective of human health. For the most part, such assertions have been related to rates of fish consumption, which is only one of several parameters of the exposure assessment component in criteria derivation. However, consideration has seldom been given to the adequacy of the entire exposure assessment component of the methodology to yield criteria that are consistent with corresponding health protection targets established in USEPA recommendations or state policies. This article discusses the level of protectiveness mandated by the Clean Water Act, USEPA's interpretation of that mandate, and the approaches USEPA recommends to achieve protection targets. An attempt is made to assess consistency between USEPA's recommended approaches and health protection targets using a quantitative assessment of the level of conservatism embodied in the default exposure parameters used in USEPA's HHWQC derivation methodology. Finally, alternative approaches that derive HHWQC that more directly correspond to specified levels of protectiveness are discussed.

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USEPA APPROACH TO ACHIEVING CWA-MANDATED PROTECTIVENESS

The CWA specifies, in a broad sense, the level of protectiveness that should be embodied in the HHWQC. It includes language such as "protect the public health and welfare," "protect public health… from any reasonably anticipated adverse effects of each pollutant," and "[not] pose an unacceptable risk to human health." In its HHWQC methodology document, USEPA notes that HHWQC are usually derived to protect the majority of the general population from chronic adverse health effects and that it

considers the target protection goal to be satisfied if the population as a whole will be adequately protected by the human health criteria when the criteria are met in ambient water (USEPA 2000a). USEPA (2004) further clarifies its overall protectiveness goals by stating that "EPA typically cannot protect every individual but rather attempts to protect individuals who represent high-end exposures (typically around the 90th percentile and above) or those who have some underlying biological sensitivity; in doing so, EPA protects the rest of the population as well."

HHWQC are traditionally derived using USEPA recommended equations (Eqns. 1, 2, and 3) that include explicit parameters for allowable risk and toxicity, and several parameters that determine exposure, including body weight, drinking water intake, fish intake, bioaccumulation, and a relative source contribution factor for noncarcinogens. Inherent to HHWQC are other assumptions not shown in the equations, referred to as implicit assumptions in this article, including duration of exposure, cooking loss, relative absorption, and the concentration of a chemical in water. The exposure assessment portion of the analyses, "BW/(DI + (ΣFIi × BAFi)," which is the primary focus of this article, is the same in all 3 equations.

For noncarcinogenic effects

$$\mathrm{RfD} \times \mathrm{RSC} \times (\mathrm{BW}/(\mathrm{DI} + (\sum \mathrm{FIi} \times \mathrm{BAFi}))), \quad (1)$$

for carcinogenic effects (nonlinear)

$$(\mathrm{POD}/\mathrm{UF}) \times \mathrm{RSC} \times (\mathrm{BW}/(\mathrm{DI} + (\sum \mathrm{FIi} \times \mathrm{BAFi}))), \text{ and} \quad (2)$$

for carcinogenic effects (linear)

$$\mathrm{RSD} \times (\mathrm{BW}/(\mathrm{DI} + (\sum \mathrm{FIi} \times \mathrm{BAFi}))), \quad (3)$$

where RfD = reference dose for noncancer effect (mg/kg-d), RSC = relative source contribution factor for sources of exposure not accounted for by DI or FIi, POD = point of departure for carcinogenic effects based on a nonlinear low-dose extrapolation, UF = uncertainty factor for carcinogenic effects based on a nonlinear low-dose extrapolation, RSD = risk-specific dose for carcinogenic effects based on a linear low-dose extrapolation, BW = human body weight (kg), DI = drinking water intake (L/day), FIi = fish intake at trophic level (TL) i (i = 2, 3, and 4), and BAFi = bioaccumulation factor at trophic level i, lipid normalized (L/kg).

USEPA (2000a) states that to derive HHWQC that are "adequately protective," it selects default parameter values that are "a combination of median values, mean values, and percentile estimates [that target] the high end of the general population."

CONSERVATISM IN INDIVIDUAL EXPOSUE ASSESSMENT PARAMETERS

Although USEPA recommends the use of parameter values that are "a combination of median values, mean values, and percentile estimates [that target] the high end of the general population" (USEPA 2000a), examination of the default values recommended by USEPA reveals that in fact, the selection of the recommended explicit exposure parameters and the assumptions that are implicit in the criteria derivation represent values taken from the upper end of the range of available data in nearly all cases. We have compared, to the extent possible, HHWQC calculated using currently recommended default exposure parameter values and those calculated using mean or median values, or, in the case of BW, more recent data.

Relative source contribution

The relative source contribution (RSC), which is used in the derivation of HHWQC for substances with noncarcinogenic effects, determines what portion of the RfD will be allocated to the consumption of water and fish from regulated waterbodies (USEPA 2000a). USEPA (2000a) provides a decision tree methodology for calculating chemical- or site-specific RSCs, notes that the information required to calculate those RSCs "should be available in most cases," and concludes that the default value of 20% "is likely to be used infrequently with the Exposure Decision Tree approach." However, rather than develop chemical-specific RSC values, USEPA (2000a) has chosen to rely on 20%, the most conservative allowable value, in its recent draft update of HHWQC (USEPA 2014a).

The California Office of Environmental Health Hazard Assessment (OEHHA) has concluded that the default use of an RSC of 20% is "unreasonably conservative for most chemicals" (Howd et al. 2004). For 22 of 57 chemicals listed by Howd et al. (2004), a RSC value greater than 20% was used in the calculation of California Public Health Goals for those chemicals in drinking water. Howd et al. (2004) also noted that "[a] default RSC of 0.2 is based on tradition, not data." Recently, the state of Florida developed specific RSC values for 21 of 35 noncarcinogenic compounds for which it derived HHWQC (FDEP 2014). Sixty-three percent of the RSC values used by Florida were greater than 0.2 (FDEP 2014).

The use of the 20% default value for RSC when a higher RSC value is warranted can result in as much as a 4-fold reduction in the HHWQC.

Body weight

The HHWQC methodology document (USEPA 2000a) recommends using a body weight (BW) of 70 kg. This weight was chosen in part because it is in the range of average weights for adults reported in several studies and in part because it is the default body weight used by USEPA's Integrated Risk Information System (IRIS) in dose extrapolation. However, in the updated edition of the Exposure Factors Handbook (USEPA 2011), USEPA recommends a mean BW of 80 kg for adults based on data from the National Health and Nutrition Examination Survey (NHANES) 1999 to 2006.

Because the toxicity parameters used in HHWQC derivation express exposure or risk as a function of body weight (e.g., mg of chemical per kg of body weight), the daily exposure that is likely to be without appreciable risk will be lower for an individual with a lower body weight than for an individual with a higher body weight. For this reason, the choice of 70 kg as the default body weight yields HHWQC that are approximately 12.5% lower than HHWQC calculated using the more representative current population mean of approximately 80 kg BW. In a recent draft proposed update of HHWQC, USEPA (2014a) acknowledged the increase in mean body weight and proposed to adopt 80 kg as the new default value for body weight.

Drinking water intake

The default drinking water intake (DI) used by USEPA in calculating HHWQC has been 2 L/d, which represents the

86th percentile for adults in a USEPA analysis of the 1994 to 1996 US Department of Agriculture (USDA) Continuing Survey of Food Intakes by Individuals (CSFII) data (USEPA 2000a). In the recently released draft update of HHWQC, USEPA (2014a) proposes increasing the default DI to 3 L/d, which is the 90th percentile for adults based on NHANES data from 2003 to 2006. The default water intake rate was selected in support of larger goals related to pollution prevention and maintenance of designated use (USEPA 2000a) and does not represent exposure that individuals are likely to receive from a regulated waterbody. A consumption rate of 2 or 3 L/d is based on estimates of direct and indirect water ingestion, primarily from municipal sources, groundwater, and bottled water, but not from untreated surface water. As USEPA (2000a) noted, it would be rare for anyone to use untreated surface water as a source of drinking water. Typically, direct consumption of untreated surface waters is limited to incidental ingestion during swimming, for which USEPA (2011) recommended upper percentile default intake rates of 120 mL/h for children and 71 mL/h for adults. Assuming the 95th percentile estimate for time spent swimming each month (181 min) (USEPA 2011) results in annual daily average incidental water consumption rates of 0.012 L/d (children) and 0.007 L/d (adults).

The effect on HHWQC of assuming 2 or 3 L/d varies according to the bioaccumulation factor (BAF) or bioconcentration factor (BCF) of the chemical. The HHWQC derivation equations consider exposures through both the direct consumption of a chemical in drinking water through the parameter "DI" and consumption of the chemical in fish tissues through the parameter "fish intake × BAF." Chemicals with high BAFs (or BCFs if BAFs are not available) will accumulate in fish tissues to a greater degree than chemicals with lower BAFs or BCFs. For chemicals with high BAFs or BCFs, the effect of drinking water intake on the ultimate HHWQC is minimal due to the much larger contribution of the "fish intake × BAF" factor in the equation. However, for substances with low BAFs or BCFs, the effect is much greater. For example, for methyl bromide, with a BCF of only 3.75 L/kg, the HHWQC calculated using a mean DI of 1 L/d (USEPA 2011) is 1.9 times greater than that calculated using 2 L/d and 2.8 times greater than when using 3 L/d.

Fish intake

The current USEPA Exposure Factors Handbook (USEPA 2011) contains summaries of a variety of surveys that have collected information on the consumption of fish, both by the general public and among specific subpopulations. The Handbook does not identify any single, specific fish consumption rate (FCR) that should be used for activities such as HHWQC derivation, but rather recommends that FCRs for the general population be based on a USEPA analysis of the 2003 to 2006 National Health and Nutrition Examination Survey (NHANES). USEPA (2011) provides a table containing per capita and "consumers only" mean and 95th percentile FCRs for "finfish," "shellfish," and "total finfish and shellfish" for all individuals, 9 different age classes, and females of reproductive age. Users are advised to select the FCR that best meets their needs from that data set.

However, USEPA (2011) also states that other relevant data on general population fish intake may be used if such data are more appropriate to the scenarios being assessed and notes that older data from the USEPA's analysis of data from the 1994 to 1996 and 1998 Continuing Survey of Food Intake by Individuals (CSFII) provide intake rates for freshwater or estuarine fish and shellfish, marine fish and shellfish, and total fish and shellfish that are not available from the NHANES analysis.

The default FCR used by USEPA in its derivation of HHWQC is 17.5 g/d, which represents an estimate of the 90th percentile per capita consumption rate of freshwater and estuarine fish for the general US adult population, based on 1994 to 1996 data from the CSFII (USEPA 2000a). In the 2014 proposed update to HHWQC, USEPA (2014a) has proposed to increase the default FCR to 22 g/d, which USEPA states represents the 90th percentile consumption of freshwater and estuarine fish for adults, based on 2003 to 2010 data from NHANES. FCR has received considerable attention during recent HHWQC revisions and reviews conducted by various states, with much discussion focused on how well the USEPA default value represents actual consumption of fish and shellfish and which fish and shellfish should be included in calculation of the FCR. Issues that have been raised include whether or not fish and shellfish harvested outside a state's jurisdiction should be included, whether or not marine species should be included, and how well the short-term food consumption surveys used by USEPA and some states as the basis for the default FCR represent long-term fish consumption rates (Polissar et al. 2012; FDEP 2014; USEPA 2014b).

The use of short-term data to represent long-term consumption of fish and shellfish. Both the CFSII and NHANES are short-term dietary intake surveys. Attempting to extrapolate long-term FCRs based on short recall period survey data presents a number of challenges. These include the potential misclassification of consumers as nonconsumers, the overestimation of upper percentile FCRs based on data collected as a snapshot in time, and the lack of consideration of variation over time (Ebert et al. 1994, WDOE 2013).

USEPA (2011) has acknowledged that short-term dietary records are problematic when attempting to estimate long-term rates of consumption, particularly for upper-bound FCR estimates. For example, in its review of NHANES 2003-2006 study data, USEPA (2011) stated that "the distribution of average daily intake rates generated using short-term data (e.g., 2-day) does not necessarily reflect the long-term distribution of average daily intake rates." Similarly, in a discussion of the limitations of a study of Michigan anglers (West et al. 1993), USEPA (2011) concluded that "because this survey only measured fish consumption over a short (1 wk) interval, the resulting distribution will not be indicative of the long-term fish consumption distribution, and the upper percentiles reported from the USEPA analysis will likely considerably overestimate the corresponding long-term percentiles." In addition, when discussing the methodology used by USDA in the CFSII, USEPA (1998) stated that "[t]he nonconsumption of finfish or shellfish by a majority of individuals, combined with consumption data from high-end consumers, resulted in a wide range of observed fish consumption. This range of fish consumption data would tend to produce distributions of fish consumption with larger variances than would be associated with a longer survey period, such as 30 days." The effect would be expected to be even larger for multiyear exposures and the lifetime consumption estimate that is implied using the currently recommended methodology for

deriving HHWQC. As a result, upper-bound fish consumption estimates based on these data are biased high and overestimate actual upper-bound consumption rates for the total population of consumers.

Some researchers have developed methodologies to address the biases associated with using short-term data to estimate long-term consumption (Tran et al. 2004, 2013; Tooze et al. 2006). In support of the state of Washington's ongoing review and revision of their HHWQC, Polissar et al. (2012) derived FCRs based on the 2003 to 2006 NHANES data using 2 methodologies. The first used only the data as collected and standard survey estimation procedures. The second used the method developed by Tooze et al. (2006), commonly referred to as the National Cancer Institute (NCI) method, to provide more accurate estimates of long-term consumption for foods like fish that tend to be consumed on a more intermittent basis. USEPA (2014b) recently acknowledged the value of the NCI approach, stating that it is "the preferred method for estimating fish consumption rates." The state of Florida, in the most recent draft Technical Support Document (TSD) developed in support of its current HHWQC revision process, also adjusted the 2003 to 2006 NHANES FCR data using the NCI method (FDEP 2014). FCRs for consumers derived using the NCI method are approximately 3-fold lower than those based on unadjusted NHANES data and would yield HHWQC that could be as much as 3-fold greater, although the magnitude of the increase is a function of the BAF or BCF.

Source of fish consumed. USEPA (2000a), in the guidance for derivation of HHWQC that was issued in 2000, encourages states and authorized tribes to derive HHWQC using FCRs based on actual data if such data are available. This may be particularly important in the case of coastal states or in interior states with limited water resources, where national data may not accurately reflect typical consumption patterns. USEPA's first preference is the use of results from fish consumption surveys of local watersheds within the state or tribal jurisdiction to establish fish consumption rates that are representative of the defined populations being addressed for the particular waterbody (USEPA 2000a). However, USEPA has recently provided additional information on what sources should be considered in the determination of FCR via a "Frequently Asked Questions" (FAQ) document (USEPA 2013). According to the FAQ, "[b]ecause the overall goal of the criteria is to allow for a consumer to safely consume from local waters the amount of fish they would normally consume from all fresh and estuarine waters, the [fish consumption rate] does include fish and shellfish from local, commercial, aquaculture, interstate, and international sources." Thus, rather than a reflection of actual consumption of fish from waterbodies that are regulated by a state's HHWQC, USEPA (2013) recommended that the fish consumption rate represent the total consumption of freshwater and estuarine fish and shellfish regardless of location of harvest, or whether or not the source is aquaculture or harvest from the wild.

The consequence of this policy decision by USEPA is that the fish consumption rate used in the calculation of HHWQC may substantially overestimate consumption of fish from regulated freshwater and estuarine waters by the majority of the population. For example, according to the National Oceanic and Atmospheric Administration (NOAA) 2011 report on "Fisheries of the United States," 91% of the seafood consumed in the United States is imported (i.e., harvested or processed outside the United States or US territorial waters), although a small portion of that was harvested in US waters, exported overseas for processing, and then reimported (NOAA 2012). Approximately 93% of shrimp, which is by far the most frequently consumed seafood in the United States, is imported (NOAA 2012).

Eight of the top 10 types of seafood consumed in the United States are either marine species or the product of aquaculture, and thus are not harvested from regulated freshwater or estuarine waters (MBA 2011). Tilapia, catfish, and pangasius, which are the most commonly consumed freshwater fish, are the products of aquaculture and, for the most part, imported from outside the United States (MBA 2011).

Excluding marine fish and shellfish from the FCR. USEPA (2000a) recommends that the fish consumption rate used to develop the HHWQC be based only on consumption of freshwater or estuarine species, with exposures via consumption of marine species being accounted for through the RSC, although coastal states and authorized tribes that believe including marine species in the total FCR is more appropriate for protecting the population of concern may do so. The CFSII (source of the current USEPA default FCR) does differentiate between freshwater, estuarine, and marine species, but NHANES (recommended source of fish consumption data in the 2011 USEPA Exposure Factors Handbook) does not. Thus, if a FCR is selected based on NHANES data, consumption of marine species will unavoidably be included in the FCR. As an alternative, USEPA (2014b) recently obtained nonpublicly available 24 h recall files with raw data from NHANES from 2007 to 2008, which it used to apportion fish intake among marine, estuarine, and freshwater sources to inform the selection of a default freshwater plus estuarine FCR for its draft update of HHWQC.

To both base its HHWQC on the most recently available FCR data, and exclude consumption of marine species when appropriate, the state of Florida, as part of its ongoing HHWQC revision process, developed a 2-part approach for adjusting FCR data. As described above, the state first adjusted 2003 to 2006 NHANES FCR data using the NCI method to more accurately reflect long-term consumption patterns. Then the NCI-NHANES FCRs were further adjusted (reduced) by applying an adjustment factor of 0.377, which is based on a ratio derived from 1994 CFSII data on combined freshwater and estuarine consumption and total consumption (freshwater, estuarine, and marine) (FDEP 2014).

Fish tissue concentration

An implicit assumption in the derivation of HHWQC is that any given HHWQC corresponds to some specific fish tissue concentration. However, the amount of any particular substance to which consumers are exposed through the consumption of fish will be affected not only by the concentration of that substance in surface waters and the quantity of fish consumed, but also by the type of fish consumed and how that fish has been prepared.

Cooking loss. The derivation of HHWQC is based on the weight of raw fish consumed and the implicit assumption that there will be no reduction in chemical concentrations in fish tissues as a result of cooking and preparation processes. However, numerous studies have shown that cooking reduces the levels of some chemicals (Skea et al. 1979; Sherer and Price

1993; Zabik et al. 1995, 1996; Zabik and Zabik 1995, 1996). For example, Zabik et al. (1995) reported that cooking significantly reduced levels of the DDT complex, dieldrin, hexachlorobenzene, the chlordane complex, toxaphene, heptachlor epoxide, and total PCBs. Similarly, Sherer and Price (1993), in a review of published studies, reported that cooking processes such as baking, broiling, microwaving, poaching, and roasting removed 20% to 30% of the PCBs whereas frying removed more than 50%.

In its development of Fish Contaminant Goals (FCGs) and Advisory Tissue Levels, the State of California uses a cooking reduction factor to account for cooking losses for some chemicals (Cal/EPA 2008). Because the concentration of PCBs and some other organic chemicals in fish are generally reduced by at least 30%, depending on cooking method, the state included a cooking reduction factor of 0.7 in the FCG equation for organic compounds, which assumes 70% of the chemical remains after cooking (Cal/EPA 2008). USEPA also recommends that cooking loss be taken into account when setting fish advisories (USEPA 2000b). Although fish advisories are typically based on fish tissue levels rather than water concentrations, the same principle applies, because any HHWQC does translate to an equivalent fish tissue concentration for that substance.

By not incorporating a chemical-specific factor to adjust for cooking loss in HHWQC derivation, exposure associated with fish consumption may be overestimated for certain organic compounds, yielding lower HHWQC.

Lipid content of fish tissue. For nonionic chemicals, the lipid content of fish tissues is an important determinant of the degree to which those chemicals will accumulate in fish tissues. As part of outlining a process for developing national BAFs, USEPA (2003a) recommended national default lipid contents of 1.9%, 2.6%, and 3.0% for tropic level 2, 3, and 4 fish, respectively. These specific values were cited (USEPA 2003a) as being the consumption-weighted means for aquatic organisms commonly consumed throughout the United States. Florida recently examined this issue using state-specific data, and determined that the consumption weighted average lipid content for Florida consumers was 1.7%.

USEPA (2014b), in its recent HHWQC draft update, used BCFs based on the assumption that all fish consumed contain 3% lipid. This implies the assumption that 100% of fish consumed are from trophic level 4, based on the previous defaults recommended by USEPA (2003a). Based on the FDEP (2014) determination that the consumption weighted average lipid content for Florida consumers was 1.7%, use of a single BCF based on 3% lipids overstates bioconcentration in fish consumed by Florida residents, and thus overstates the risk associated with consuming fish caught in Florida (FDEP 2014). Similarly, the assumption of 3% lipid content likely overstates bioconcentration and risk for the general public, given that several of the most commonly consumed types of seafood in the United States (MBA 2011) are lower trophic level species (e.g., shrimp, tilapia, crab). For example, the most commonly consumed seafood in the United States is shrimp (MBA 2011), which has a lipid content of 1% to 2% (FDEP 2014).

Exposure duration

Exposure duration is an implicit element in the derivation of HHWQC for carcinogens and a value of 70 y, or an approximate lifetime, is assumed. Although average lifetimes may be approximated by 70 y, few people will drink and fish only one set of waters for an entire lifetime. Choosing to assume a 70 y exposure duration may be appropriate in cases where a chemical is ubiquitous in the environment (e.g., chemicals for which atmospheric deposition is the dominant mechanism for entry into surface waters) and it could reasonably be assumed that ingestion of drinking water and locally caught fish from all freshwater locations would lead to similar levels of exposure. There is little evidence, however, supporting the ubiquity of most substances for which HHWQC have been established.

However, many individuals move one or more times during their lifetimes and, as a result of those moves, may change their fishing locations and the sources of the fish they consume, thus changing their potential exposure profile. For example, a Pew Research Center study (Taylor et al. 2008) found that 63% of Americans have moved to a new community at least once in their lives and 43% of Americans have lived in 2 or more different states. In addition, it is likely that most anglers will not fish every year of their lives. Health issues and other demands, like work and family obligations, will likely result in no fishing activities or reduced fishing activities during certain periods of time that they live in a given area.

It is difficult to quantify the impacts of mobility and fishing habits on actual duration of exposure, especially because it seems reasonable to suspect that tribal, subsistence, and low income fishers (high level consumers) might be less mobile relative to the general population. However, the assumption of a 70 y exposure duration for all members of the population clearly adds conservatism to the derivation of HHWQC.

Surface water concentration

Implicit in the derivation of HHWQC is the assumption that both the water column and fish tissue concentrations exist at their maximum allowed for the entire implied 70 y exposure duration. In reality, water column concentrations vary over time and space. The assumption that water concentrations are always equal to the HHWQC and fish tissue concentrations are equal to those expected following continuous exposure to the HHWQC adds an additional layer of protectiveness because, as a practical matter, regulations governing water quality in the United States would not allow most regulated chemicals to persist in a water body at the HHQWC concentration for such an extended period. Exceptions to this may be chemicals whose primary sources are beyond the reach of water quality regulatory programs (e.g., airborne Hg, naturally-occurring As).

USEPA's Impaired Waters and Total Maximum Daily Load Program provides guidance to states concerning when waters are to be listed as impaired under the terms of the Clean Water Act. The USEPA guidance does not provide specific recommendations for identifying stream impairments due to exceedances of HHWQC, and state impaired stream listing methodologies often do not include specific provisions. In general, states seem to adopt 1 of 2 approaches: a specific limit on the number of exceedances of water quality limits for some fixed duration or the "10% Rule." Alabama Department of Environmental Management (2012), for example, considers listing a waterbody if "[t]here is more than one exceedance of a particular toxic pollutant criterion in [the] previous six years."

West Virginia Department of Environmental Protection (2012), on the other hand, applies the "10% Rule," stating that "if an ample data set exists and exceedances of…human health protection criteria occur more than 10 percent of the time, the water is considered to be impaired."

No matter which approach is adopted, average concentrations must be lower than the HHWQC to ensure that exceedances do not occur. This situation is acknowledged in the USEPA (2003b) guidance for listing impaired surface waters, which states that "[u]sing the '10% rule' to interpret data for comparison with chronic WQC will often be consistent with such WQC because it is unlikely to lead to the conclusion that water conditions are better than WQC when in fact, they are not." Based on the 10% rule, it would be more accurate to identify the HHWQC as the 90th percentile value in a distribution of water column concentrations existing over 70 y rather than a concentration to which living organisms are continuously exposed.

COMPOUNDED CONSERVATISM IN DERIVATION OF HHWQC

Most of the USEPA-recommended default values representing exposure parameters and implicit assumptions used in the derivation of HHWQC are selected from the upper percentiles of available data ranges (USEPA 2000a). The overall consequences of such choices have been acknowledged and addressed by regulatory agencies and individual researchers. For example, in its Cancer Risk Assessment Guidelines USEPA (2005) cautioned that combining multiple overly conservative assumptions is likely to lead to risk estimates that are above the 99th percentile of the distribution of potential risk and may be of limited use to decision makers. Similarly, Lichtenberg (2010) noted that the use of conservative default parameters introduces an upward bias into estimates of risk, and concluded that "the numbers generated by such procedures cannot really be thought of as estimates of risk, because they bear only a tenuous relationship to the probability that individuals will experience adverse health consequences or to the expected prevalence of adverse health consequences in the population."

A sense of what compounded conservatism means in the context of HHWQC derivation may be gained by estimating the proportion of the total population composed of individuals exposed at the levels represented by the default parameter values. Ten percent of the general population consumes the default 17.5 g/d or more of freshwater or estuarine fish (USEPA 2000a). Fourteen percent of the population consumes the default 2 L/d or more of water (USEPA 2000a). However, only 1.4% of the population is likely to consume at least 17.5 g/d of fish and drink at least 2 L/d of water.

This shows the effect of compounded conservatism for just 2 exposure assumptions. When other factors that affect the exposure assumptions are considered, such as that most of the fish consumed in the United States are imported and that it is unlikely that any individual will use untreated surface water as a regular source of drinking water, it is clear that HHWQC are based on exposures that are relevant for much less than 1% of the population, which is substantially more conservative than the goals (90th percentile, 10^{-6} risk level) recommended by USEPA.

Although the toxicity factors used in derivation of HHWQC have not been a focus of this article, they also contribute to the compounding of conservatism in HHWQC. Consider, for example, the UFs that are used by USEPA in the derivation of RfDs, which are in turn used in the calculation of HHWQC for substances with noncarcinogenic effects and substances such as chloroform, which has a nonlinear dose–response for carcinogenic effects. In RfD derivation, UFs are used to adjust the selected dose level from the underlying toxicological study to account for scientific uncertainties related to variations in sensitivity among humans (UF_H), extrapolation from animal studies to humans (UF_A), extrapolation from less than chronic (i.e., subchronic) no observed adverse effect levels (NOAELs) to chronic NOAELs (UF_S) or use of a lowest observed adverse effect level (LOAEL) rather than a NOAEL (UF_L) to define the RfD (USEPA 2000c). A default UF of 10 is typically used for each source of uncertainty noted above, although in some cases, a reduced UF of 3 is applied when available data or scientific understanding indicate that there is more certainty as a result of the availability of more data or a greater understanding of mode of action (USEPA 2000c). As noted by Gaylor and Kodell (2000), multiplying several uncertainty factors, each of which represents an upper bound estimate, results in an unnecessary compounding of conservatism, because it is unlikely that each uncertainty factor needs to be simultaneously at the maximum value. Similarly, Swartout et al. (1998) pointed out that the multiplication of conservative UFs acts to "repeat" conservative assumptions at each step of the process. For example, Swartout et al. (1998) concluded that default UFs of 100, 1000, and 3000, for application of 2, 3, and 4 UFs, respectively, could be replaced with UFs of 51, 234, and 1040 and still maintain a 95th percentile level.

USEPA (2000a) recommends the use of parameter values that are a combination of medians, means, and upper percentile estimates that target the high end of the general population to derive HHWQC. In actual practice, however, the selection of values representing explicit exposure parameters and the assumptions embodied by implicit parameters in the criteria derivation methodology represent upper-bound values in nearly all cases, resulting in HHWQC that greatly exceed the level of protectiveness identified by USEPA (2000a) as the basis for the HHWQC.

ALTERNATIVE APPROACHES

HHWQC that are more closely aligned with USEPA's stated protectiveness goals might be derived by selecting default parameter values from distributions that more accurately reflect current data or better represent long-term behavior, such as using NCI method-adjusted NHANES data on fish consumption. In the recently released draft update of HHWQC, USEPA (2014a) has adopted this approach. For example, the agency has proposed to increase the default value for BW to 80 kg and adjust fish consumption data to reduce bias due to the use of short-term consumption data as a surrogate for long-term fish consumption rates (USEPA 2014a).

Another alternative would be to replace some of the upper-end default values with mean and median values, and explicitly address some of the implicit parameters by selecting specific values for those parameters from the published scientific literature and regional studies. For some exposure parameters, sufficient data are available to provide complete distributions from which mean, median, or alternative percentile values may be selected for use. For example, the most recent Exposure Factors Handbook (USEPA 2011) contains complete data distributions, based on large national surveys, for drinking water intake. The primary obstacle to application of this approach is a lack of guidance on which upper-end percentile default

exposure parameter values should be replaced with mean or median values, or accepted guidance upon which such choices should be based.

Another option would be to replace the current deterministic approach to HHWQC derivation with a probabilistic approach, such as that proposed by the state of Florida (FDEP 2014). In the Florida approach, distributions rather than point estimates were used for body weight, drinking water intake, and fish consumption rate (FDEP 2014). FDEP (2014) explained their preference for the probabilistic approach:

"Reliance on point values discards valuable information on variability within population. Furthermore, use of the deterministic approach has led to a focus on the wrong endpoints. The focus of criteria development should not be selection of a fish consumption rate or any other point value, but rather on setting criteria at the concentration of a pollutant in water that is not expected to pose a significant risk to human health over a lifetime. The probabilistic approach allows the focus to be shifted back to the true concern, specifically, the risk of exceeding the RfD or risk-specific dose (10^{-6}/cancer slope factor, RSD)."

Under Florida's probabilistic approach, body weight, drinking water intake, and fish consumption rate data are inserted into the equation as probability distributions based on variability in the target population (FDEP 2014). The analysis treats the exposure distributions as random variables and allows for an evaluation of risk to both the entire population and to higher risk subpopulations (FDEP 2014). This allows the risk assessor to specify the desired risk management endpoint and then demonstrate that the endpoint is met by the HHWQC. For example, for carcinogens, FDEP (2014) proposed HHWQC ensuring that average Floridians will be protected at greater than the 10^{-6} risk level, regular (weekly) consumers of Florida fish will protected at the 10^{-5} level, and that all Floridians, including subsistence fishers, will be protected at better than 10^{-4}. For noncarcinogens, FDEP (2014) calculated a Hazard Quotient (HQ) (total intake from fish and drinking water divided by the RfD, and then multiplied by body weight), then proposed HHWQC that achieve a HQ of 1.0 at the 90th percentile, which ensures that exposures to a large majority of the population will not exceed the RfD.

CONCLUSION

Despite USEPA (2000a) guidance to use "combinations of median values, mean values and percentile estimates that target the high end of the general population" when deriving HHWQC for the protection of public health, most states and tribes have calculated criteria using values from the upper ends of distributions for the exposure parameters. Also, several parameters, for which upper percentiles or maximums are employed, are implicit in the derivation methodology (e.g., assuming zero loss due to cooking) and contribute additional conservatism. Such conservative selections for these exposure parameters, combined with conservative toxicity parameters, can result in criteria that are substantially more protective than implied by USEPA's recommended health protection goals because of the compounding effect that occurs when multiple conservative factors are combined. This situation may be mitigated by thoughtful selection of exposure parameter values when using a deterministic approach, or by using a probabilistic approach based on data distributions for many of these parameters.

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ATTACHMENT J

Probabilistic Approach to Deriving Ambient Water Quality Criteria White Paper

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Probabilistic Approach to Deriving Ambient Water Quality Criteria White Paper

August 13, 2014

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Probabilistic Approach to Deriving Ambient Water Quality Criteria White Paper

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Table of Contents

Acronyms and Abbreviations

ASF	age sensitivity factor
AT_c	averaging time for carcinogenic effects
AT_{nc}	averaging time for noncarcinogenic effects
AWQC	ambient water quality criteria
BAF	bioaccumulation factor
BW	body weight
California EPA	California Environmental Protection Agency
CL	cooking loss
CLF	catch location factor
CSF	cancer slope factor
DI	drinking water intake
DOC	dissolved organic content
ED	exposure duration
ELCR	excess lifetime cancer risk
EMAP	Environmental Monitoring and Assessment Program
EPI	Estimation Program Interface
FCR	fish consumption rate

FDEP	Florida Department of Environmental Protection
g/day	grams per day
HQ	hazard quotient
kg	kilogram
L/day	liters per day
LHF	life history factor
MCA	Monte Carlo Analysis
NAWQA	National Water Quality Assessment Program
NHANES	National Health and Nutrition Examination Survey
ODEQ	Oregon Department of Environmental Quality
POC	particulate organic content
POD	points of departure
PRA	probabilistic risk assessment
RBA_w	relative bioavailability, water
RBA_f	relative bioavailability, fish
RfD	reference dose
RME	reasonable maximum exposure
RSC	relative source contribution
TELCR	target excesslifetime cancer risk
THQ	target hazard quotient
TSD	Technical Support Document
ug/L	micrograms per liter
USEPA	United States Environmental Protection Agency
USGS	Unites States Geological Survey
WDOE	Washington Department of Ecology

Executive Summary

To date, national ambient water quality criteria (AWQC), including those proposed by the United States Environmental Protection Agency (USEPA) in May 2014, have been established using deterministic risk assessment methods using almost exclusively upper bound or maximum values for variables that govern human exposure and toxicity of the compounds that are being regulated. This leads to a phenomenon that has been termed "compounded conservatism." The effect is to overestimate potential risk associated with exposure to chemicals in surface waters and, as a result, to develop AWQC that are more stringent than necessary to achieve USEPA's stated risk management goals. USEPA recognized this potential in its 2000 AWQC methodology yet uses repeated conservative assumptions to derive the proposed 2014 AWQC. USEPA has also recognized the ability of probabilistic risk assessments (PRA) to characterize the level of conservatism in risk assessments and has identified conditions for which PRAs are applicable and useful. The setting of national AWQC meets those conditions. This paper describes how PRA can be used to set AWQC and includes three case studies to demonstrate that the level of protection associated with USEPA's proposed AWQC is greater, in some cases substantially greater, than implied by USEPA's stated risk management goals. The case studies document other advantages of PRA over the deterministic approach. One such advantage is the ability to use as inputs to the derivation of AWQC all data associated with a particular variable (e.g., fish consumption, water ingestion, body weight) instead of selecting a single value as is necessary for deterministic assessments. Use of all data allows inclusion of all segments of the population in the derivation of AWQC and focuses the discussion surrounding the derivation of AWQC on the overall protectiveness of the AWQC and not on individual parameters used to derive the AWQC as has often been the case historically (e.g., selection of a single fish consumption rate). A second advantage is increased transparency regarding the protectiveness of the AWQC. In its 2000 AWQC methodology USEPA acknowledges that a deterministic approach precludes a quantitative assessment of the level of protection afforded different segments of the population. Because USEPA and others have now developed distributions for most of the key variables that determine exposure and risk to chemicals in surface water, PRA can be used to estimate the distribution of risk for the entire population and AWQC can be developed that afford specified levels of protection to different segments of the population.

1. Introduction

Traditionally, ambient water quality criteria (AWQC) have been derived by regulatory agencies using deterministic risk assessment methods (e.g., USEPA 2000). Those methods assign a single value (from a range of possible values) to each parameter in an equation that yields an AWQC. Parameters include those that represent an exposure scenario, toxicity, and allowable risk level. Some view the selection of the allowable risk level as the only risk management decision in the setting of AWQC. That is incorrect. Selecting a single value from a range entails an element of subjectivity and is often a topic of debate (Finley and Paustenbach 1994, Burmaster 1995). In the context of setting criteria, selection of a single input value from a range of values represents a risk management decision or policy choice. Unfortunately, the effect of the choice relative to the intended risk management goal is not always apparent.

Because regulatory agencies tend to err on the side of protecting public health, the derivation process typically incorporates the selection of conservative values (i.e., high-end or maximum values) for several parameters establishing the AWQC (USEPA 1989, 1991a, 2011). Collectively, using multiple conservative assumptions for AWQC may be far more protective than necessary to meet a risk management goal. This phenomenon of greater conservatism embodied by the whole than the conservatism of each individual part is referred to as "compounded conservatism" (Nichols and Zeckauser 1986). When using a deterministic risk assessment approach, it is impossible to discern the degree to which AWQC are more protective than implied by the risk management goal and the actual level of protection afforded different segments of the population. Probabilistic risk assessment (PRA) is an alternative to the traditional deterministic risk assessment methods. It uses the range of values for a particular parameter thereby reducing the need for risk management decisions tied to each parameter. Because the outcome of PRA is a distribution of risk, it makes the risk management decisions (i.e., the level of protection afforded different segments of the population) more transparent within the AWQC derivation process.

The concept of probabilistic assessment is not a new one; the United States Environmental Protection Agency (USEPA) has issued formal guidance for conducting probabilistic risk assessments (USEPA 2001) as well as a white paper encouraging the use of probabilistic risk assessment in decision making (USEPA 2014a,b). However, many agencies, including USEPA, have continued to use the traditional deterministic approach to deriving AWQC, despite criticism that the deterministic approach is overly conservative and can lead to unrealistic estimates of risk (Nichols and Zeckauser 1986, Burmaster and Harris 1993). Furthermore, although USEPA guidance recommends

basing deterministic risk assessments on exposure assumptions representing a combination of median values, mean values, and upper percentile estimates to avoid compounded conservatism (USEPA 2005), agencies continue to derive AWQC using conservative upper-percentile defaults for most of the derivation parameters (e.g., USEPA 2014c).

The USEPA Risk Assessment Forum states that PRA can "facilitate better characterization of uncertainty and improve the overall transparency and quality of EPA assessments" and describes the following situations in which PRA is useful (USEPA 2014a,b).

1. A specified target level of protection in a population is identified by the manager (e.g., the 95th percentile), and it is necessary to demonstrate that this goal is met.
2. Significant equity or environmental justice issues are raised by variation in risks among the exposed population of concern.
3. Screening-level point estimates of risk are higher than an accepted level of concern.
4. Uncertainty in some aspect of the risk assessment is high, and decisions are contentious or have large resource implications.
5. Specific critical risk estimates and assumptions point to different management options.
6. The scientific rigor and quality of the assessment is critical to the credibility of the EPA decision.
7. When a screening-level deterministic risk assessment indicates that risks are possibly higher than a level of concern and a more refined assessment is needed.
8. When the consequences of using point estimates of risk are unacceptably high.
9. When significant equity or environmental justice issues are raised by interindividual variability.
10. When exploring the impact of the probability distributions of the data, model and scenario uncertainties as well as variability together to compare potential decision alternatives.

Many of the situations described by USEPA (2014a,b) apply directly to the establishment of national AWQC. Recently, the benefits of using the probabilistic approach to derive AWQC have been recognized by state regulatory agencies. For example, the Florida Department of Environmental Protection (FDEP) has developed proposed state criteria using probabilistic methods that allow the State to demonstrate all segments of the population, including high end consumers, are protected at appropriate acceptable risk levels.

The purpose of this white paper is to describe the probabilistic approach to deriving AWQC. In contrast to the deterministic approach, the probabilistic approach accounts for variability within populations and uncertainty surrounding parameters by allowing one or more of the exposure parameters to be defined as distributions of potential values (i.e., probability density functions). The paper describes the benefits of PRA compared to the traditional deterministic approach, presents three case studies demonstrating those benefits, and documents the effect of compounded conservatism in USEPA's proposed AWQC which leads to substantially more stringent AWQC than necessary to achieve USEPA's stated risk management goals.

2. Background

The general AWQC derivation process uses equations that account for the key exposure pathways (i.e., consumption of water and fish). Deterministic AWQC are derived using equations that include both exposure and toxicity parameters combined with a risk management goal (i.e., an acceptable risk level). Probabilistic AWQC are derived by using these same equations, combined with distributions for one or more parameters representing the inherent variability in a population's physical characteristics and behaviors, or the uncertainty surrounding a parameter, to generate a distribution of risk. The AWQC derived using probabilistic methods is the water concentration that has associated with it a distribution of potential risk that meets (i.e., does not exceed) the risk management goal(s) selected by the regulatory agency. In some cases, a regulatory agency may select a single risk management goal. For example, a regulatory agency might require that the hazard quotient (HQ) for the 90^{th} percentile of the population be equal to or less than 1.0. Alternatively, a regulatory agency may select multiple risk management goals that need to be met by an AWQC. For example, that the 50^{th} percentile of the population (the median) must have an excess lifetime cancer risk (ELCR) equal to or less than $1x10^{-5}$ and that the 99th percentile of the population must have an ELCR equal to or less than $1x10^{-4}$.

2.1 Monte Carlo Analysis

Monte Carlo Analysis (MCA) is used to generate a distribution of risk when one or more input variables are defined as probability distributions. This technique has been widely used in engineering, finance, and insurance as an alternative to solving equations with probability distributions analytically, which is mathematically complex (USEPA 2001). MCA is easily accomplished using commercial software (e.g., @Risk or Crystal Ball). The computer randomly selects input values from each probability distribution and solves the equation to calculate risk; this process is called an iteration.

Typically, a large number of iterations are performed (e.g., 10,000 or more). One set of iterations is called a simulation. After the simulation is complete, the resulting risk estimates form a distribution of potential risk that can be compared to the target risk management goal(s). The MCA process is shown schematically in **Figure 1**.

2.2 Equations

AWQC are derived using the fundamental human health risk equations employed by (USEPA 2014c). The USEPA equation for chemicals with noncarcinogenic endpoints is:

$$AWQC = \frac{THQ \; x \; BW \; x \; RSC \; x \; RfD}{DI + \sum_2^4 (FCR_i \; x \; BAF_i)} \quad \textbf{(Equation 1)}$$

The USEPA equation for chemicals with carcinogenic endpoints is:

$$AWQC = \frac{TELCR \; x \; BW}{\left[DI + \sum_2^4 (FCR_i \; x \; BAF_i)\right] \; x \; CSF} \quad \textbf{(Equation 2)}$$

Where:

THQ = target hazard quotient (unitless);
TELCR = target excess lifetime cancer risk (unitless);
DI = drinking water intake (L/day);
FCR_i = trophic level-specific fish consumption rate (kg/day);
BAF_i = trophic level-specific bioaccumulation factor (L/kg tissue);
BW = body weight (kg);
RSC = relative source contribution (unitless);
RfD = reference dose (mg/kg-day); and
CSF = cancer slope factor $(mg/kg\text{-}day)^{-1}$.

In addition to the parameters explicitly listed in the USEPA equations, additional implicit parameters also affect the characterization of risk and can be included in the AWQC derivation equations. The expanded equation for chemicals with noncarcinogenic health endpoints is:

$$AWQC = \frac{THQ \; x \; BW \; x \; AT_{nc} \; x \; RSC \; x \; RfD}{\left[(RBA_w \; x \; DI) + \left(RBA_f \; x \; \sum_2^4 (FCR_i \; x \; CLF_i \; x \; LHF_i \; x \; BAF_i) \; x \; (1 - CL)\right)\right] \; x \; ED} \quad \textbf{(Equation 3)}$$

The expanded equation for chemicals with carcinogenic health endpoints is:

$$AWQC = \frac{TELCR\ x\ BW\ x\ AT_c}{\left[(RBA_w\ x\ DI) + \left(RBA_f\ x\ \sum_2^4 (FCR_i\ x\ CLF_i\ x\ LHF_i\ x\ BAF_i)\ x\ (1-CL)\right)\right]\ x\ ED\ x\ CSF} \quad \textbf{(Equation 4)}$$

Where the additional implicit parameters include:

RBA_w = relative bioavailability, water (unitless);
RBA_f = relative bioavailability, fish (unitless);
CLF_i = trophic level-specific catch location factor (unitless);
LHF_i = trophic level-specific life history factor (unitless);
CL = cooking loss (unitless);
ED = exposure duration (years);
AT_{nc} = averaging time for noncarcinogenic effects (years); and
AT_c = averaging time for carcinogenic effects (years).

When AWQC are derived using Equations 1 and 2, these implicit parameters are each effectively incorporated at their highest possible value, thereby resulting in AWQC with additional layers of conservatism. For example, excluding the relative bioavailability and cooking loss terms assumes that the chemical in water and fish is 100% bioavailable and that none of the chemical in fish is lost during the cooking process. Excluding the exposure duration and averaging time terms assumes that exposure duration is equal to averaging time – in other words, it assumes an exposed individual will live in the same place for their entire life (e.g., 70 years) and that 100% of the water and fish they consume during those 70 years will come from the regulated water body. Excluding the catch location factor and life history factor terms assumes that 100% of fish consumed are caught from local regulated waters and spend the entirety of their lives in the same regulated waters. While USEPA has indirectly accounted for life history by excluding marine and a portion of anadromous fish from the overall fish consumption rate (e.g., USEPA 2014c), the remaining implicit parameters are often left unaddressed. These parameters should be included in the AWQC derivation equations to make the level of conservatism embodied in AWQC clear.

2.3 Sources of Data

Developing parameter distributions for use in a probabilistic assessment has at times historically been viewed as a challenge due to a perceived lack of robust sources of data. However, numerous sources of robust statistical data now exist and can be used to characterize the variability and uncertainty in parameters that determine AWQC. Simply put, if sufficient data exist to establish a distribution from which a point estimate representing a specific percentile can be selected (e.g., the 95th), then the data should

be available to define a full probability distribution (USEPA 2014b). Sources for national exposure data include:

- **USEPA Exposure Factors Handbook (USEPA 2011)** – Provides a summary of statistical data describing a number of behavioral and physiological factors commonly used in human health risk assessment, including but not limited to drinking water intake, fish consumption rate, body weight, and exposure duration; and

- **USEPA Estimated Fish Consumption Rates for the U.S. Population and Selected Subpopulations (USEPA 2014d)** – Provides an analysis of long-term average fish consumption rates for the general U.S. population using data from the National Health and Nutrition Examination Survey (NHANES) 2003-2010.

State-specific or regional data may also be available to characterize various aspects of exposure. Some examples include:

- **Oregon Department of Environmental Quality (ODEQ) Guidance for Use of Probabilistic Analysis in Human Health Risk Assessments (ODEQ 1998)** – Provides distributions for numerous exposure factors commonly used in risk assessment;

- **Washington Department of Ecology (WDOE) Fish Consumption Rates Technical Support Document: A Review of Data and Information about Fish Consumption in Washington (WDOE 2013)** – Provides an evaluation of available information on fish consumption in Washington State; and

- **FDEP Draft Technical Support Document: Derivation of Human Health-Based Criteria and Risk Impact Statement (FDEP 2014)** – Provides national and state-specific distributions used to derive AWQC for the State of Florida.

2.4 Using PRA to Derive AWQC

The equations presented in Section 2.2 are sometimes referred to as “backward” risk equations. That is, USEPA uses equations that predict an allowable water concentration (i.e., the AWQC) based on an allowable risk, exposure scenario, and toxicity. These equations are typically used for deterministic calculation of risk-based acceptable media concentrations (e.g., AWQC or preliminary remediation goals at waste sites).

As described by Burmaster et al. (1995) and Ferson (1996), deriving AWQC using probabilistic methods requires "forward" equations. That is, the equations estimate risk from a chemical concentration, exposure scenario, and toxicity. In essence, the forward equation will yield a distribution of risks dependent on several inputs that are also distributions. If the equation is "flipped" to solve for one of the inputs, the resulting distribution and the original input distribution may have similar means, but the spread of the distributions will be different. Because the tails of a distribution (e.g., highly exposed individuals) are often of interest when setting acceptable risk or acceptable media concentrations, this disparity has marked effects on the outcome of the calculation. Therefore, USEPA recommends using forward equations when conducting probabilistic assessments to avoid the mathematical limitations associated with back-calculation (USEPA 2001).

For probabilistic derivation of AWQC, the process of estimating risk by selecting from the input point estimates or distributions is repeated until the number of desired iterations (e.g., 100,000 iterations for the case studies presented herein) is complete. As long as one or more of the input parameters are distributions, the final output of a simulation will be a distribution of risks associated with a particular concentration of a chemical in water. If the estimate of risk matches the desired risk management goal(s), the chemical concentration that was used to generate the output is the AWQC.

Typically, multiple simulations are required to derive probabilistic AWQC. Two methods can be used to develop the AWQC: the iterative approach and systematic linear derivation. Both require that allowable risk goals be established for at least one, and possibly several, statistics of the risk distribution (e.g., the mean, median, 90th percentile, 95th percentile).

- In the **iterative approach** (shown schematically in **Figure 2**), a water concentration is selected and the resulting risk distribution is compared to risk management goal(s). If one or more goals is exceeded, the process is repeated using alternative chemical concentrations until a concentration is identified that results in a risk distribution that meets all risk management goals. That concentration is the AWQC.

- The **systematic linear derivation** approach is recommended by USEPA (2001) as a "shortcut" for the trial-and-error method when using probabilistic methods to calculate risk-based acceptable media concentrations. Typically, simulations are run at three alternative chemical concentrations. The estimated risks at the percentile of the risk distribution corresponding to the risk management goal

versus the chemical concentration used for each simulation are plotted (**Figure 3**). (The example in **Figure 3** is for the carcinogenic endpoint, but a similar process would be used for the non-cancer endpoint.) A least-squares linear regression line is fit to the paired excess lifetime cancer risk and concentrations for each statistic of the distribution corresponding to the risk management goal. The equation for each statistic is used to solve for the chemical concentration that corresponds to the risk management goal (e.g., allowable risk level) for that statistic. If only one risk management goal needs to be met (e.g., excess lifetime cancer risk at the 90^{th} percentile must be equal to or less than $1x10^{-5}$), the concentration that meets that goal is the AWQC. When more than one risk management goal needs to be met, the AWQC is the lowest of the concentrations derived from all of the risk management goals. The example shown in Figure 3 requires that two risk management goals be met. In this example the mean of the risk distribution must be equal to or less than $1x10^{-6}$ which occurs at a concentration of 9.9 micrograms per liter (ug/L) and the 90^{th} percentile must be equal to or less than $1x10^{-5}$ which occurs at 44 ug/L. In this case the AWQC would be set at 9.9 ug/L such that both goals are met. Commonly, risk associated with one of the descriptors of the risk distribution is below its risk management goal. In this case, while the risk to the average member of the population is equal to the risk management goal of $1x10^{-6}$ at a concentration of 9.9 ug/L the risk associated with the 90^{th} percentile at that same concentration is approximately $2x10^{-6}$, which is about five times lower (more stringent) than required by the risk management goal of $1x10^{-5}$ for the 90^{th} percentile.

3. Key Concepts of Probabilistic Approach

The probabilistic approach to deriving AWQC offers numerous advantages over the deterministic approach. Perhaps the clearest advantage of the probabilistic approach is that it provides risk managers with more information than the traditional deterministic approach. Three case studies are presented below demonstrating how variables can be represented by distributions of values capturing not only observed variability but also uncertainty associated with exposure and risk. Two additional considerations, the potential correlation between variables and the uncertainty associated with the tails of the risk distribution, are also discussed. The case studies illustrate that the ability to use as inputs to the derivation of AWQC all data associated with a particular parameter that affects exposure (e.g., fish consumption, water ingestion, body weight) increases transparency about the protectiveness of AWQC and helps focus stakeholders on the overall process and the ultimate public health protection afforded by AWQC and not any single assumption used to derive AWQC.

3.1 Case Study: Variability of Exposure Parameters

To illustrate the transparency afforded by the probabilistic approach, a case study is presented using USEPA's May 2014 draft updated AWQC for benzo(a)pyrene, chlordane, and benzene (i.e., 0.00077, 0.0000068, and 0.45 ug/L, respectively, for intake of water and fish). According to USEPA, these criteria are "meant to be protective of human health for the *general* [emphasis added] adult population from an increased cancer risk…at a 10^{-6} or 1 in 1,000,000 risk level" (USEPA 2014e,f,g). To better understand the range of potential risk associated with these criteria, distributions were initially defined for three exposure parameters: body weight, drinking water intake, and fish consumption rate. Using the same datasets used by USEPA to select point estimates for these parameters, distributions were developed using @Risk (**Table 1**). These distributions represent all ranges of behavior, including highly exposed members of the population. For example, the drinking water intake distribution assumes that 1% of the population ingests more than 5 liters of untreated surface water for every day of their lifetime. While the maximum drinking water intake rate varies between simulations, it is approximately 15 liters per day (L/day) on average over a lifetime. Similarly the fish consumption distribution assumes that 1% of the population consumes more than 58 grams of fish for every day of their lifetime. The maximum consumption rate is consistently greater than USEPA's subsistence consumption rate of 142 grams per day (g/day) (USEPA 2000) and is, on average over a lifetime, approximately 184 g/day. In other words, the PRA includes people who are assumed to eat approximately 184 grams of fish per day, every day of the year, for every year of their assumed 70 year lifetime.

A probabilistic assessment was conducted using these three distributions along with the point estimates selected by USEPA for the remaining input parameters. The results of this analysis show that the median (50^{th} percentile) excess lifetime cancer risk ranges from $2.3x10^{-7}$ to $5.1x10^{-7}$ for the three chemicals. Similarly, the mean excess lifetime cancer risk ranges from $4.4x10^{-7}$ to $5.9x10^{-7}$. Excess lifetime cancer risk for the 90^{th} percentile is approximately $1.0x10^{-6}$ for all chemicals (**Figure 4**). On average, the maximum risk is slightly less than $1x10^{-5}$ for all chemicals. The shape of the risk distribution varies between chemicals because the relative contribution of the drinking water and fish consumption pathways varies between chemicals. Exposure associated with the drinking water pathway will be identical for all chemicals because the distribution of water consumption is the same for all chemicals. However, exposure associated with the fish consumption pathway will vary. chemicals with higher bioaccumulation factors (BAFs) (e.g., benzo(a)pyrene and chlordane) will have a higher risk contribution from the fish consumption pathway than chemicals with lower

BAFs (e.g., benzene), altering the shape of the cumulative risk distribution associated with drinking water and fish combined.

The distributions of risk, based just on input distributions for body weight, water ingestion and fish consumption, find that the excess lifetime cancer risk of the average member of the population is more than two-fold lower than the stated goal of protecting the general adult population at a risk level of $1x10^{-6}$, assuming the definition of the "general adult population" is the average member of the population. If the "general adult population" is assumed to be the median (50^{th} percentile) member, then the level of protection associated with the proposed criteria are closer to 4-fold more stringent than USEPA's stated goal. Additionally, the proposed criteria are substantially more stringent than necessary to be consistent with USEPA's 2000 methodology, which states "EPA believes that both 10^{-6} and 10^{-5} may be acceptable for the general population and that highly exposed populations should not exceed a 10^{-4} risk level" (USEPA 2000). As discussed above, the exposure distributions include high-end behaviors for both water ingestion and fish consumption, and people with body weights of less than 50 kilograms. Thus, highly exposed populations are included and shown to have excess lifetime cancer risk of about $1x10^{-5}$, or about an order of magnitude (10-fold) less than suggested by USEPA (2000).

These PRA results indicate that the proposed AWQC for benzo(a)pyrene, chlordane, and benzene, based on consideration of just these three exposure variables alone, could be increased by at least four-fold, and perhaps as much as 10-fold and still have the potential risks associated with the general adult population fall within USEPA's stated goal of $1x10^{-6}$ and $1x10^{-5}$ being acceptable risk levels for the general population and to limit the excess lifetime cancer risk of highly exposed populations to less than $1x10^{-4}$.

As shown above in the equations used to estimate AWQC, many parameters in addition to bodyweight, fish consumption and water ingestion affect exposure and risk and the numerical value of AWQC. Because USEPA uses high-end or maximum values for many of these other parameters, expanding the PRA to incorporate distributions for one or more of these other parameters is likely to demonstrate that USEPA's proposed AWQC are even more conservative than suggested by using distributions for just bodyweight, fish consumption and water ingestion. The effect of incorporating distributions for two other parameters is presented and discussed below.

3.2 Case Study: Variability of Bioaccumulation

In addition to the three exposure parameters evaluated in Section 3.1, distributions can be included for other parameters as well. For example, numerous conservative assumptions are used to develop the trophic level-specific BAFs used by USEPA to derive the proposed AWQC. If distributions are used to represent the input parameters that determine the BAFs, a distribution of predicted BAFs can be generated. BAFs are only one of several other exposure parameters that could be represented using distributions (e.g., cooking loss, chemical concentration in surface water).

Expanding the case study, distributions were developed for the trophic level-specific benzo(a)pyrene and chlordane BAFs. First, distributions were developed for several parameters that affect BAFs. Next, distributions were developed for the BAFs associated with each trophic level using the equations presented in the Estimation Program Interface (EPI) Suite BCFBAF^{TM} model (USEPA 2012).

Distributions of lipid content in edible portions of trophic level 2, 3, and 4 fish were developed using the observations obtained from the online Environmental Monitoring and Assessment Program (EMAP) and Storet databases maintained by USEPA (**Table 2**). EMAP was designed to store data for use in ecological monitoring and risk assessment. The Storet database includes water quality and toxicity obtained from government agencies, Indian Tribes, volunteer organizations, academia, and other organizations. It provides a large quantity of lipid data from several regions throughout the U.S. and for numerous species and thus enables the development of national fish lipid distributions based on trophic level. Lipid data were subdivided into trophic levels 2, 3, and 4, based on trophic levels classified in USEPA (2014d). Specific species not included in the USEPA (2014d) trophic level classification were obtained from Froese and Pauley (2014). Trophic level values from Froese and Pauley (2014) were provided to one decimal place and were rounded to the next trophic level at decimal values of x.5 and higher. Distributions were then developed for proportion lipid in each of the three trophic levels using @Risk (**Table 2**).

Distributions of dissolved organic content (DOC) and particulate organic content (POC) were also developed using data obtained from the United States Geological Survey (USGS) National Water Quality Assessment Program (NAWQA). This monitoring program, started in 1991, collects chemical and physical water quality data from 51 study sites nationwide and stores this information in an online database (USGS 2001). Distributions were developed for both DOC and POC using @Risk (**Table 2**).

Distributions for lipid content of trophic level 1 organisms, organism weight, and temperature were developed by selecting a range of values for each parameter. For lipid content of lowest trophic level organisms and organism weight, the range was defined as half the USEPA default at the low end and two times the USEPA default at the high end. Lipid content of lowest trophic level organisms therefore was defined as a uniform distribution ranging from 0.005 to 0.02. Organism weight ranged from 0.048 to 0.192 kilograms (kg), 0.092 to 0.368 kg, and 0.765 to 3.06 kg for trophic level 2, 3, and 4 organisms, respectively (**Table 2**). Temperature was defined as a uniform distribution ranging from 5 to 28^{o}C, a range selected to reflect the range of surface water temperatures across the United States (**Table 2**).

An Excel spreadsheet version of the EPI Suite BCFBAF^{TM} model was created using the equations and assumptions listed in the BCFBAF^{TM} Help File. An MCA was conducted using the three trophic level-specific lipid distributions along with the point estimates defined by USEPA for the remaining input parameters. In this way, distributions were developed for bioaccumulation in each of the three trophic levels using @Risk (**Table 2**). Most of the BAFs included in the distribution of BAFs are lower than the BAFs used by USEPA to derive the proposed AWQC.

Using the exposure parameter distributions described in Section 3.1, along with the distributions developed for bioaccumulation, a PRA was again conducted using the draft updated AWQC for benzo(a)pyrene and chlordane. The results of this analysis show that incorporating variability for an additional element – in this case, bioaccumulation – not only increases variability in the risk distribution but reduces risk estimates even further. The effect is relatively small for benzo(a)pyrene (**Figure 5**) but larger for chlordane (**Figure 6**). The 95th percentile chlordane excess lifetime cancer risk drops from 1.5x10^{-6} to 6.5x10^{-7} and the mean drops from 4.4x10^{-7} to 1.8x10^{-7}. On average, the maximum risk drops from approximately 9x10^{-6} to 5x10^{-6}. These results demonstrate that the proposed criteria are even more stringent than suggested by a PRA based on distributions for only three exposure parameters and that the proposed AWQC for chlordane could perhaps be increased by as much a 20 times (from 0.0000068 ug/L to 0.00014 ug/L) and still remain protective of the general population as well as highly exposed populations.

3.3 Case Study: Uncertainty in Toxicity

Generally, the distributions used in probabilistic risk assessments are limited to parameters that determine exposure because of a reluctance on the part of USEPA to incorporate uncertainty and variability associated with toxicity assumptions in PRA.

However, distributions can also be developed for parameters used to estimate toxicity [i.e., the reference dose (RfD) or cancer slope factor (CSF)]. Given that these are selected to overpredict response for a given exposure, for example because cancer slope factors are an upper bound estimate of response as opposed to the best estimate of response, using a distribution for toxicity estimates is likely to lead to a further decrease in potential risk for the general adult population. While the distributions for most exposure parameters represent primarily variability among the population for that particular parameter, the distributions representing toxicity reflect variability in response between animals but also uncertainty about the extrapolation of response in the human population based on studies in animals. Depending upon chemical, that uncertainty has the potential to be large.

To illustrate the effect of toxicity uncertainty, a distribution of CSFs associated with oral exposure to benzo(a)pyrene was developed. Benzo(a)pyrene was selected as one example for this final case study, though toxicity distributions could be developed for most other chemicals using distributions of CSFs for the cancer endpoint and distributions of RfDs for the non-cancer endpoint.

Numerous rodent bioassays report tumorigenicity results associated with oral exposure to benzo(a)pyrene, mainly in tissues of the alimentary tract (USEPA 2013). Of these studies, the rat bioassay by Kroese et al. (2001) and the female mouse bioassay by Beland and Culp (1998) provided the best available dose-response data for extrapolating to lifetime cancer risk. Both studies were conducted in accordance with Good Laboratory Practices, included controls, three dose levels, sufficient numbers of test animals per dose group, appropriate exposure durations, and included histopathological evaluation in multiple tissue types. Other bioassays which have been used previously by USEPA to estimate CSFs (USEPA 1991b), such as Brune et al. (1981), Neal and Rigdon (1967), and Chouroulinkov et al. (1967), were not considered in this analysis due to shortcomings in experimental design compared to the Kroese et al. (2001) and Beland and Culp (1998) studies.

USEPA (2013), California EPA (2010), and ARCADIS (2013) relied on the tumorigenicity data reported by Kroese et al. (2001) and Beland and Culp (1998) to calculate CSFs. USEPA (2013) developed dose-response relationships for the combined incidence of forestomach, esophagus, tongue, and larynx squamous cell tumors from Beland and Culp (1998) and for each tumor response site reported by Kroese et al. (2001). The multistage-Weibull model, which incorporates time-to-tumor incidence, was used to estimate points of departure (POD) as the lower 95% bound benchmark doses at the 10% extra risk level. CSFs were then calculated using linear

low-dose extrapolation as it was assumed that benzo(a)pyrene has a mutagenic mode of action (USEPA 2013). California EPA (2010) modeled the combined incidence of tumors of the esophagus, forestomach or tongue from Beland and Culp (1998) and the liver and combined forestomach and oral cavity adenomas or carcinomas from Kroese et al. (2001) using the multistage-Weibull time-to-tumor model. CSFs were then calculated using linear low-dose extrapolation from the POD, which was set to the lower 95% confidence bound for the dose associated with a 10% increased cancer risk. ARCADIS (2013) independently modeled the combined esophageal papilloma and carcinoma data from Beland and Culp (1998) using a multistage cancer model, where the POD was estimated as the lower bound 95% confidence interval on the dose level associated with a 10% extra cancer risk, and using linear low-dose extrapolation to calculate the CSF.

ARCADIS used the esophageal tissue tumor incidence data from Beland and Culp (1998) to calculate the benzo(a)pyrene CSF. USEPA and California EPA also relied on data from Beland and Culp (1998) to calculate CSFs, but only after combining tumor incidence data for multiple organs and tissue types, including the forestomach. The forestomach is an organ in rodents that holds ingested food before entry into the stomach. When benzo(a)pyrene-incorporated food is fed to rodents, benzo(a)pyrene has a longer contact time with the forestomach membranes than it does with the membranes of the stomach or intestines. Humans do not have a forestomach or other organ that holds food prior to entry to the stomach. Thus, forestomach tumorigenicity data is not relevant to human health assessments. However, benzo(a)pyrene in food travels through the esophagus quickly following ingestion in both rodents and humans, resulting in similar food-tissue contact times. USEPA has argued that esophageal tissue is similar in nature to rodent forestomach tissue and hence, rodent forestomach tumor data is relevant to human health risk assessment. In many rodent studies, only forestomach tumor data are available. However, for this example, rodent esophageal tissue data were used to estimate human health risks.

Calculating CSFs based on the results from multiple studies provides a means of aggregating sources of response variability and uncertainty. The Kroese et al. (2001) rat bioassay and Beland and Culp (1998) mouse bioassays each display within-study variability in dose-response and subsequent CSF estimates. This is attributed to physiological differences between sexes in the Kroese et al. (2001) study, the approach used to group tissue-specific responses and/or tumors with differing histopathologies, and the mathematical modeling procedures used to estimate CSFs. In addition, interspecies differences in sensitivity between rats and mice, differences between exposing test animals to benzo(a)pyrene via gavage or diet, differences in

treatment designs, and differences in study protocols between laboratories produce between-study variability in CSF estimates. Taken together, the studies included here capture uncertainties associated with 1) the relevance of using rodent/tissue-specific tumorigenicity responses in the forestomach, an organ that humans do not possess, to estimate human risks, 2) the range of CSF magnitudes calculated using different target organ and response-site groupings, and 3) extrapolating from tumorigenicity data in rodents to risks in humans.

The final distribution of CSFs was developed using values calculated by USEPA (2013), California EPA (2010), and ARCADIS-US (2013), which all relied on data from the Kroese et al. (2001) and Beland and Culp (1998) bioassays (**Table 3**). The input values derived from Beland and Culp (1998) were weighted more heavily in MCA (66%) than the input values calculated from the Kroese et al. (2001) bioassay (33%). This was done to reflect USEPA's selection of the Beland and Culp (1998) alimentary tract-based CSF as the most sensitive tumorigenic end-point in their recent toxicological review of benzo(a)pyrene (USEPA 2013).

The CSF distribution includes seven CSFs adjusted using age sensitivity factors (ASFs) for early lifestage exposure and seven CSFs without this adjustment. The use of ASF-adjusted CSFs introduces another layer of uncertainty. All of the exposure assumptions used by USEPA to derive the proposed benzo(a)pyrene AWQC are representative of adults or assume a lifetime of exposure. Body weight, drinking water intake, and fish consumption rate are all derived from data for adults 21 years of age or older. Because exposure duration and averaging time are not explicitly included in the equation used to derive USEPA's proposed AWQC, the implicit assumption is a duration of exposure equal to a full lifetime. Exposure assumptions that are representative of adults may not be representative of children. Therefore, using a toxicity benchmark adjusted for the potential increased sensitivity of children may not be appropriate when estimating the potential risks associated with adult lifetime exposures. To capture this uncertainty, the distribution includes CSFs with and without the ASF adjustment.

Using the exposure parameter and bioaccumulation distributions described in Sections 3.1 and 3.2, along with the distribution developed for toxicity, a 2-dimensional MCA (2D-MCA) was conducted using the draft updated AWQC for benzo(a)pyrene. The 2D-MCA used nested computational loops (i.e., 100 outer loop simulations and 5,000 inner loop iterations) where the exposure and bioaccumulation distributions were repeatedly sampled for each iteration but the toxicity distribution was only sampled once for each simulation. The 2D-MCA was conducted this way to assess how the risk distribution

might shift upward or downward with varying assumptions for toxicity. The 5% and 95% confidence intervals (i.e., the lower 5% and upper 95% confidence bounds) associated with the best estimate (i.e., arithmetic mean) of potential risk were plotted alongside the individual simulation results (**Figure 7**).

The results of this assessment show that the uncertainty associated with benzo(a)pyrene toxicity causes risk estimates to vary by more than an order of magnitude from the high to low end. For example, the upper bound estimate of the 90th percentile risk (i.e., 1.0x10^{-6}) is over ten times greater than the lower bound estimate (i.e., 7.2x10^{-8}) (**Figure 7**). These PRA results indicate that depending upon the level of confidence associated with the estimated risk at a particular percentile of the distribution of risk, the proposed AWQC for benzo(a)pyrene could potentially be increased by several fold and still meet USEPA's stated risk management goals. For example, the best estimate of risk associated with the distribution of cancer slope factors is approximately three-fold lower than the upper 95th percentile confidence bound (**Figure 7**).

3.4 Correlation Between Variables

In addition to concerns about the adequacy of data to develop robust input distributions, other concerns have been raised about PRA. Those include the effect of failing to account for correlations between input variables and model uncertainty. As discussed above, robust data are now available to develop input distributions for key variables. The effect of correlation is discussed below, as is model uncertainty.

Correlation is a measure of dependence between random variables. In the case of probabilistic risk assessment, correlation refers to the strength of association between exposure parameters. For example, it has been suggested that the probabilistic approach to deriving AWQC should take into account the possibility that larger people (i.e., those with higher body weights) may be more likely to consume larger amounts of both water and fish. In its July 2012 *Technical Support Document: Derivation of Human Health Criteria and Risk Assessment* (TSD), FDEP accounted for both of these correlations in its calculations (FDEP 2012).

To evaluate the implications of accounting for correlations in the derivation of AWQC, FDEP's July 2012 methodology, selected as a readily available example of correlations between exposure parameters, was applied to a single chemical. Using the distributions defined by FDEP in its July 2012 TSD for drinking water intake, body weight, fish consumption rate, and fraction lipid, potential ELCR distributions were

generated for benzo(a)pyrene at USEPA's 2009 national recommended water quality criterion level of 0.0038 ug/L (USEPA 2009). Two simulations were run, each using 100,000 Monte Carlo iterations. One simulation accounted for correlations between body weight and both drinking water intake and fish consumption rate, as defined in FDEP's July 2012 TSD. The second simulation used the same input distributions but did not account for any correlations between variables.

The results of this evaluation show that accounting for correlation between variables reduces the probability of extreme high or low exposure estimates (e.g., a very large person consuming a very small amount of fish or vice versa). The overall spread of the ELCR distribution when accounting for correlations is reduced compared to the ELCR distribution when not accounting for correlations (**Figure 8**). For example, the 5th percentile ELCR when accounting for correlations is higher ($2.5x10^{-7}$ versus $2.2x10^{-7}$) and the 95th percentile ELCR is lower ($1.0x10^{-6}$ versus $1.1x10^{-6}$). That being said, the 50th percentile of the two distributions ($5.0x10^{-7}$) is virtually the same. Therefore, when deriving AWQC using the probabilistic approach, not accounting for correlations appears to be a conservative approach, at least in the case of the assumed positive correlation of ingestion of water or fish and body weight. Increasing the spread of the risk distribution in both directions effectively increases the risk estimates at the low- and high-end percentiles of the distribution, thereby lowering the resultant AWQC when risk management goals are focused on these percentiles (**Table 4**).

3.5 Instability of Extreme Percentiles

When establishing risk management criteria, an important consideration is the decreasing stability of risk estimates at extreme percentiles. USEPA recommends the 90th to 99.9th percentiles as the reasonable maximum exposure (RME) range for decision-making purposes (USEPA 2001). However, caution should be exercised when relying on extreme upper-end percentiles for risk management purposes. These higher percentiles (e.g., the 99.9th) tend to be highly uncertain due to the limited number of data points in these ranges.

To illustrate this point, a 2D-MCA was used to estimate the uncertainty associated with random selection of input values from predefined input distributions (i.e., model uncertainty). For continuity, the input distributions from FDEP's July 2012 TSD were once again used to assess potential ELCR for benzo(a)pyrene in this analysis (FDEP 2012). Because the selection of input values for each iteration is random, the resulting estimate of potential risk associated with each iteration is unique. Consequently, the risk distributions resulting from each set of simulation will be very similar but will not be

identical. The 2D-MCA used nested computational loops (i.e., a 2D-MCA with 100 outer loop simulations and 5,000 inner loop iterations) to repeatedly sample the input distributions to quantify the effect of the random selection of input values and estimate the 5% and 95% confidence intervals (i.e., the lower 5% and upper 95% confidence bounds) associated with the best estimate (i.e., arithmetic mean) of potential risk resulting from that random selection. The results of this analysis show that there is a high degree of certainty associated with risk estimates at the 50th percentile (i.e., there is a narrow confidence interval associated with risk estimates at the 50th percentile) (**Figure 9**). The degree of certainty decreases slightly (i.e., the confidence interval widens) at the 95th percentile and decreases significantly at the 99.9th percentile.

4. Discussion and Conclusions

The case studies have demonstrated that sufficient information is available for several key exposure parameters to develop input distributions that represent the range of exposures in the population and that those can be incorporated in a PRA to develop a distribution of potential risks for the population. Though presented only for benzo(a)pyrene in this white paper, sufficient information about the toxicity of most compounds is available to establish distributions for toxicity parameters as well. Evaluation of some of the more commonly cited concerns about PRA (i.e., correlation between input variables, model uncertainty) indicates that those are unlikely to have a large effect on the outcome and interpretation of the results of a PRA, though it is clear from the evaluation of model uncertainty that the highest and lowest percentiles of the risk distribution (i.e., below the 1st and above the 99th percentiles, the extreme tails) are less stable than the majority of the distribution and that setting AWQC based on such percentiles should be undertaken with great caution, or not at all.

The case studies have also confirmed that a deterministic risk assessment approach that used primarily high-end assumptions and one or two central tendency assumptions results in AWQC that are substantially more stringent than implied by the risk management goals upon which the criteria are based (e.g., in the case of USEPA's 2014 proposed AWQC, protecting the general adult population at a 1x10^{-6} allowable risk level). The degree to which the stated risk management goals are exceeded depends upon the chemical but also on the risk management goals used. PRA makes the level of protection far more transparent than do deterministic risk assessment methods. This is perhaps the greatest value of PRA; it allows for a much clearer separation of risk assessment and risk management than is possible with deterministic risk assessment methods.

The distribution of risk developed using the probabilistic approach is determined primarily by the distributions defined for each input parameter. (As indicated in this white paper, model uncertainty also makes a small contribution to the range of risk.) So long as the input distributions are based on sound science and data, and capture the range of variability and uncertainty in each parameter – both at the high end low end, the resulting distribution will represent an unbiased characterization of potential risk. Conversely, the risk estimated using the deterministic approach is determined entirely by the selection of point estimates for each parameter and the policy decisions embodied therein. By the very nature of the deterministic approach, therefore, risk assessment and risk management are intertwined. The probabilistic approach helps separate the two.

The derivation of AWQC using the probabilistic approach depends on a combination of the science (which is more robust) and risk management assumptions (which are more transparent). Using the same input distributions, two risk managers could derive two entirely different sets of AWQC, varying only in the target risk level and target population percentile chosen. Risk managers must explicitly choose to protect certain segments of the population, recognizing that the entire population cannot be afforded "equal protection" because highly exposed individuals will, by definition, always have a higher exposure and thus higher risk.

To illustrate the importance of risk management assumptions, three hypothetical AWQC for benzo(a)pyrene were derived using the same input distributions but different risk management criteria. All three hypothetical AWQC used the distributions for body weight, drinking water intake, and fish consumption rate described in Section 3.1. All three hypothetical AWQC used a target risk of one in a million (i.e., $1x10^{-6}$); however, one targeted the mean of the distribution, one targeted the 90th percentile, and one targeted the 99th percentile. Despite using the same exposure parameter assumptions in all three cases, the resulting AWQC targeting the mean, 90th percentile, and 99th percentile (i.e., 0.0017, 0.00076, and 0.00028 ug/L, respectively) vary by nearly an order of magnitude from the high to low end (**Figure 10**). This hypothetical example demonstrates how great an effect the risk management assumptions have on the resulting AWQC.

In some cases, states have elected to select the equivalent of an extreme upper percentile of the risk distribution and apply a stringent risk management goal to such an extreme percentile. One example is Oregon's selection of a 175 g/day fish consumption rate and an allowable cancer risk of $1x10^{-6}$. The effect of these risk management choices can be estimated using the case studies presented above. If one

were to assume Oregon's consumption rate of 175 g/day represents the maximum risk within the case study, then the 90th percentile and median risks are approximately 1x10^{-7} and 3x10^{-8}, respectively. This is about 10 times more stringent than the risk management goal Oregon uses for the application of PRA at waste sites [i.e, protecting the 90th percentile at 1x10^{-6} (ODEQ 1998)].

In conclusion, the probabilistic approach to deriving AWQC makes both risk assessment and risk management more transparent. Robust statistical data are readily available for key exposure parameters and programs are available to adopt the PRA approach. By allowing inclusion of all segments of the population in the derivation of AWQC, the probabilistic approach focuses the discussion surrounding the derivation of AWQC on the overall protectiveness of the AWQC and not on individual parameters used to derive the AWQC. Regulators using the probabilistic approach can make explicit and clear choices about risk management and can describe what level of protection is afforded across the entire population of exposed individuals.

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Tables

Table 1. Exposure Factor Distributions

Percentile	Body Weight (kg)	Drinking Water Intake (L/day)	Fish Consumption Rate (g/day)
Distribution Type	**Weibull**	**Weibull**	**Pearson V**
Mean	80.547 [a]	1.7227	9.319
1%	48.8	0.1096	1.295
5%	53.522	0.3583	1.374
10%	57.326	0.552	1.533
15%	60.428	0.7034	1.747
20%	63.196	0.8354	2.013
25%	65.777	0.957	2.334
30%	68.252	1.0729	2.714
35%	70.672	1.1863	3.16
40%	73.076	1.2993	3.681
45%	75.497	1.414	4.289
50%	77.966	1.5323	5.002
55%	80.518	1.6562	5.842
60%	83.19	1.788	6.84
65%	86.033	1.9309	8.041
70%	89.111	2.0894	9.514
75%	92.523	2.2699	11.366
80%	96.425	2.4833	13.782
85%	101.099	2.7498	17.12
90%	107.157	3.1151 [b]	22.213 [c]
95%	116.456	3.7259	31.853
99%	134.757	5.1474	58.056

Notes:

g/day = grams per day

kg = kilogram

L/day = liters per day

[a] Consistent with mean body weight of 80 kg used to derive May 2014 draft updated AWQC.

[b] Consistent with 90th percentile drinking water intake of 3 L/day used to derive May 2014 draft updated AWQC.

[c] Consistent with 90th percentile fish consumption rate of 22 g/day used to derive May 2014 draft updated AWQC.

Table 2. Bioaccumulation Factor Input and Output Distributions

Percentile	Proportion Lipid				Organism Weight (kg)			Temperature (°C)	Dissolved Organic Content (mg/L)	Particulate Organic Content (mg/L)
	Trophic Level 1	Trophic Level 2	Trophic Level 3	Trophic Level 4	Trophic Level 2	Trophic Level 3	Trophic Level 4			
USEPA Default	**0.01**	**0.0598**	**0.0685**	**0.107**	**0.096**	**0.184**	**1.53**	**10**	**0.5**	**0.5**
Distribution Type	**Uniform**	**Log-Logistic**	**Pearson V**	**Inverse Gaussian**	**Uniform**	**Uniform**	**Uniform**	**Uniform**	**Log-Logistic**	**Lognormal**
Mean	0.0125	0.0096	0.0107	0.0135	0.120	0.230	1.913	16.5	5.22	1.66
1%	0.0052	0.0008	0.0014	0.0015	0.049	0.095	0.788	5.23	0.51	0.06
5%	0.0058	0.0016	0.0024	0.0022	0.055	0.106	0.880	6.15	1.04	0.11
10%	0.0065	0.0022	0.0031	0.0029	0.062	0.120	0.995	7.3	1.43	0.16
15%	0.0073	0.0028	0.0037	0.0034	0.070	0.133	1.109	8.45	1.75	0.22
20%	0.0080	0.0032	0.0043	0.0040	0.077	0.147	1.224	9.6	2.04	0.27
25%	0.0088	0.0037	0.0048	0.0046	0.084	0.161	1.339	10.75	2.31	0.33
30%	0.0095	0.0042	0.0053	0.0052	0.091	0.175	1.454	11.9	2.57	0.39
35%	0.0103	0.0047	0.0059	0.0059	0.098	0.189	1.568	13.05	2.84	0.46
40%	0.0110	0.0052	0.0064	0.0067	0.106	0.202	1.683	14.2	3.12	0.55
45%	0.0118	0.0057	0.0071	0.0075	0.113	0.216	1.798	15.35	3.41	0.64
50%	0.0125	0.0063	0.0077	0.0084	0.120	0.230	1.913	16.5	3.72	0.74
55%	0.0133	0.0069	0.0085	0.0095	0.127	0.244	2.027	17.65	4.06	0.87
60%	0.0140	0.0076	0.0093	0.0108	0.134	0.258	2.142	18.8	4.44	1.02
65%	0.0148	0.0084	0.0102	0.0123	0.142	0.271	2.257	19.95	4.88	1.20
70%	0.0155	0.0094	0.0113	0.0141	0.149	0.285	2.372	21.1	5.39	1.43
75%	0.0163	0.0106	0.0127	0.0164	0.156	0.299	2.486	22.25	6.01	1.73
80%	0.0170	0.0122	0.0145	0.0193	0.163	0.313	2.601	23.4	6.82	2.14
85%	0.0178	0.0145	0.0169	0.0235	0.170	0.327	2.716	24.55	7.94	2.74
90%	0.0185	0.0182	0.0206	0.0298	0.178	0.340	2.831	25.7	9.72	3.74
95%	0.0193	0.0262	0.0282	0.0419	0.185	0.354	2.945	26.85	13.49	5.94
99%	0.0199	0.0589	0.0535	0.0750	0.191	0.365	3.037	27.77	27.80	14.19

Notes:
kg = kilogram
L/kg tissue = liters per kilogram of tissue
mg/L = milligrams per liter
USEPA = United States Environmental Protection Agency

Table 2. Bioaccumulation Factor Input and Output Distributions

Percentile	Benzo(a)pyrene Bioaccumulation Factor (L/kg tissue)			Chlordane Bioaccumulation Factor (L/kg tissue)		
	Trophic Level 2	Trophic Level 3	Trophic Level 4	Trophic Level 2	Trophic Level 3	Trophic Level 4
USEPA Default	**2,736**	**983.7**	**395.6**	**688,200**	**1,318,000**	**3,205,000**
Distribution Type	**Inverse Gaussian**	**Pearson V**	**Weibull**	**Inverse Gaussian**	**Inverse Gaussian**	**Gamma**
Mean	3,011	913	264	230,601	505,167	1,398,021
1%	492	182	48	10,661	29,712	146,548
5%	845	320	107	30,247	79,235	244,432
10%	1,097	407	142	46,645	118,954	342,579
15%	1,301	473	166	60,880	152,594	433,601
20%	1,484	530	186	74,458	184,085	522,643
25%	1,659	582	202	87,995	214,987	612,087
30%	1,831	631	217	101,862	246,192	703,488
35%	2,004	680	231	116,348	278,356	798,122
40%	2,181	728	243	131,719	312,057	897,209
45%	2,366	777	256	148,261	347,885	1,002,064
50%	2,561	827	267	166,307	386,507	1,114,218
55%	2,770	881	279	186,274	428,738	1,235,568
60%	2,998	937	291	208,712	475,638	1,368,588
65%	3,250	999	303	234,385	528,664	1,516,667
70%	3,535	1,068	315	264,412	589,930	1,684,694
75%	3,868	1,147	328	300,537	662,713	1,880,171
80%	4,269	1,240	343	345,714	752,532	2,115,576
85%	4,780	1,358	359	405,564	869,822	2,414,166
90%	5,495	1,520	379	492,942	1,038,314	2,827,871
95%	6,713	1,796	408	649,971	1,335,167	3,521,359
99%	9,562	2,451	459	1,045,555	2,063,083	5,091,150

Notes:
kg = kilogram
L/kg tissue = liters per kilogram of tissue
mg/L = milligrams per liter
USEPA = United States Environmental Protection Agency

Table 3. Benzo(a)pyrene Cancer Slope Factor Distribution

Study	Distribution Weight (%)	Modeling group	CSF value $(mg/kg\text{-}d)^{-1}$	ASF adjusted CSF value $(mg/kg\text{-}d)^{-1}$ [a]	Basis
Beland and Culp (1998)	66	USEPA (2013)	1.0	1.7	Combined forestomach, esophagus, tongue, larynx (alimentary tract): squamous cell tumors
		California EPA (2010)	1.7	2.9	Combined forestomach, esophagus, tongue tumors
		ARCADIS US (2013)	0.2	0.3	Esophageal tumors (papillomas and carcinomas)
Kroese et al., (2001)	33	USEPA (2013), High - Male	0.4	0.7	Combined forestomach and oral cavity, squamous cell tumors
		USEPA (2013), High - Female	0.3	0.5	Combined forestomach and oral cavity, squamous cell tumors
		California EPA (2010), High - Male	0.36	0.6	Combined forestomach and oral cavity, squamous cell tumors
		California EPA (2010), High - Female	0.33	0.6	Combined forestomach and oral cavity, squamous cell tumors

Notes:
ASF = age sensitivity factor
CSF = cancer slope factor
mg/kg-d = milligrams per kilogram per day
[a] The same ASF used by California EPA (2010) of 1.7x was used here.

Table 4. Hypothetical AWQC Derived for Benzo(a)pyrene With and Without Correlations

Percentile of Population Protected at ELCR of $1.0x10^{-6}$	AWQC (ug/L)	
	Without Correlations [a]	With Correlations [b]
50th	0.0076	0.0076
75th	0.0055	0.0058
90th	0.0042	0.0045

Notes:
AWQC = ambient water quality criteria
ELCR = excess lifetime cancer risk
ug/L = micrograms per liter
[a] No correlations defined between exposure parameters.
[b] Correlations defined between body weight and both drinking water intake and fish consumption rate.

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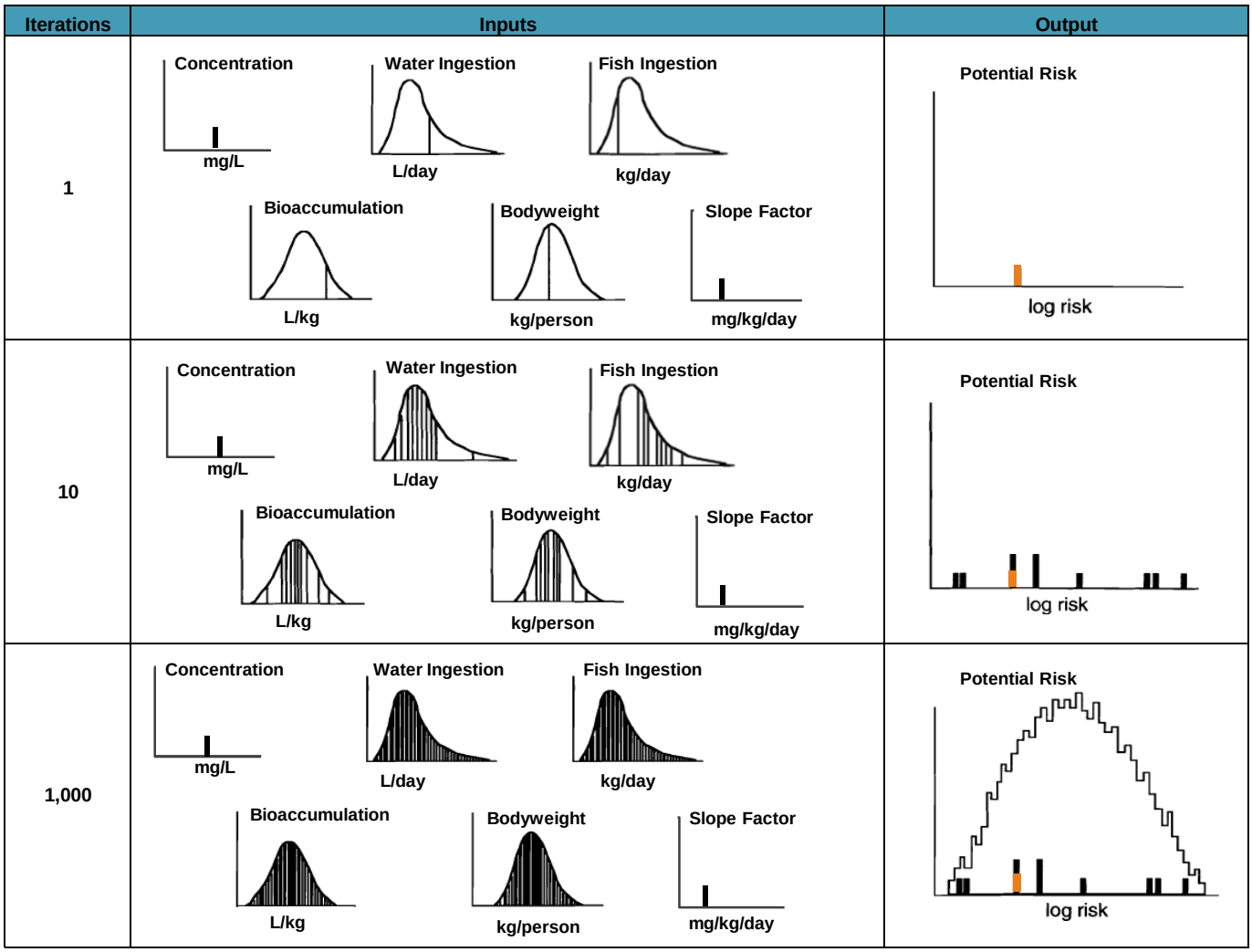
Figures



PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

SCHEMATIC OF MONTE CARLO ANALYSIS

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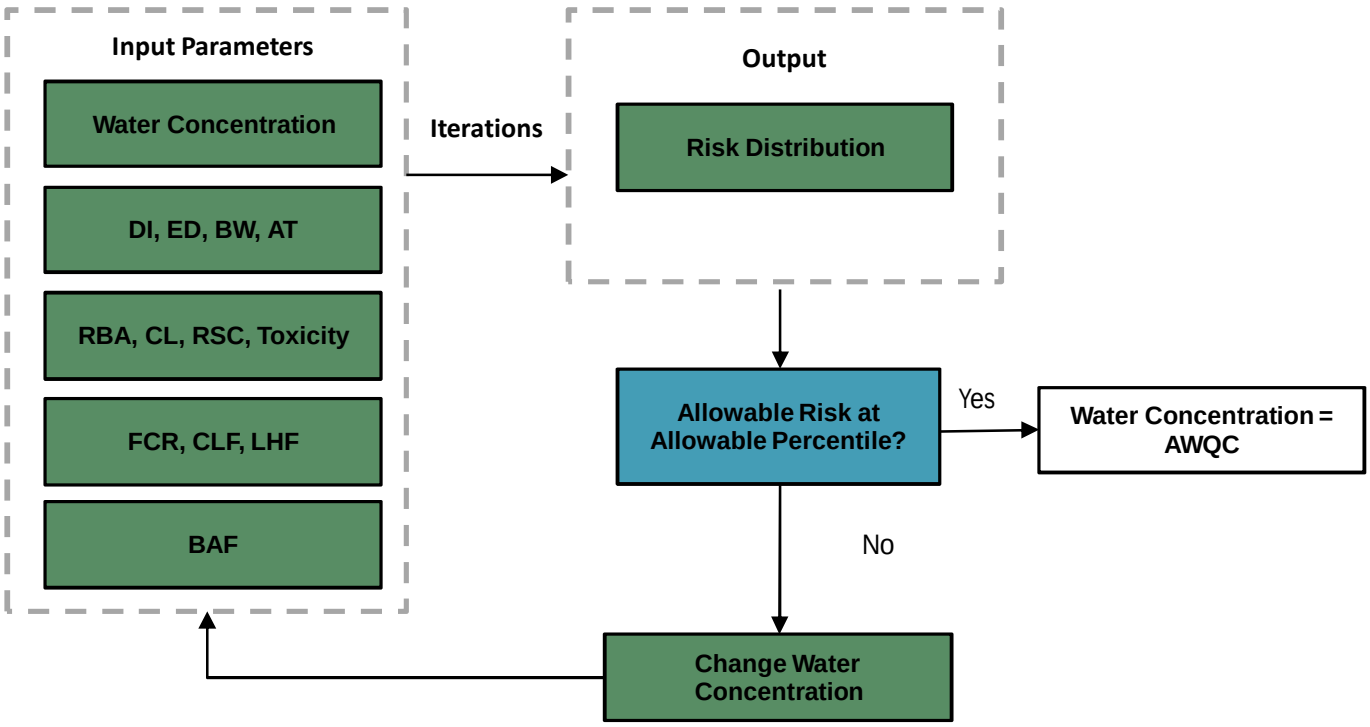
FIGURE 1



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SCHEMATIC OF ITERATIVE APPROACH

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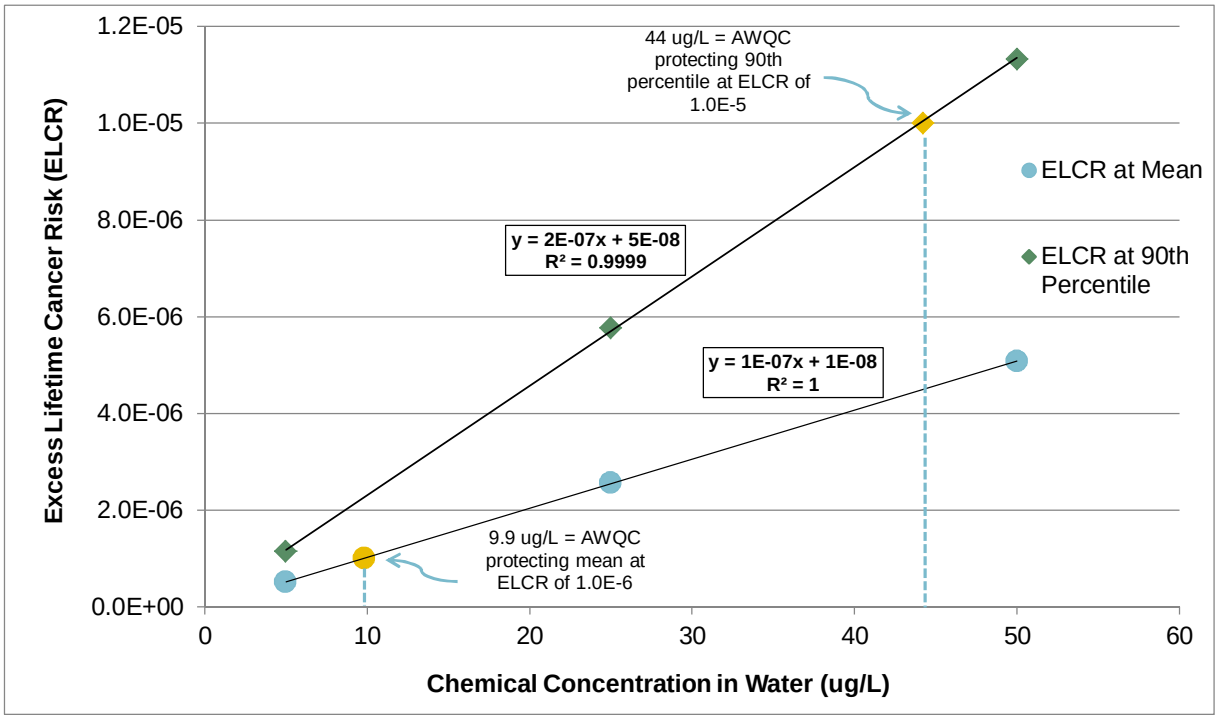
FIGURE 2



PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

SCHEMATIC OF SYSTEMATIC LINEAR DERIVATION APPROACH

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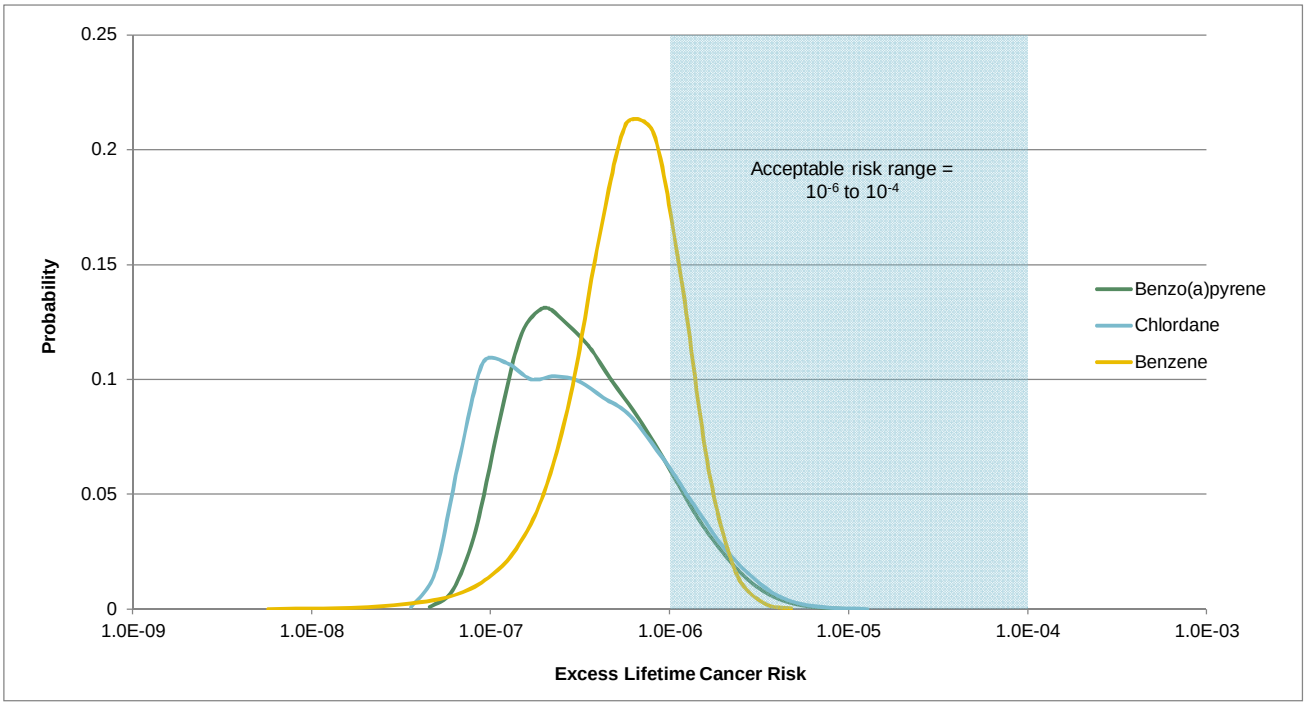
FIGURE 3



Chemical	Excess Lifetime Cancer Risk			
	Mean	Median	90th Percentile	95th Percentile
Benzo(a)pyrene	4.6E-07	2.7E-07	1.0E-06	1.5E-06
Chlordane	4.4E-07	2.3E-07	1.1E-06	1.5E-06
Benzene	5.9E-07	5.1E-07	1.1E-06	1.3E-06

PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

CASE STUDY: BENZO(A)PYRENE, CHLORDANE, AND BENZENE EXCESS LIFETIME CANCER RISK

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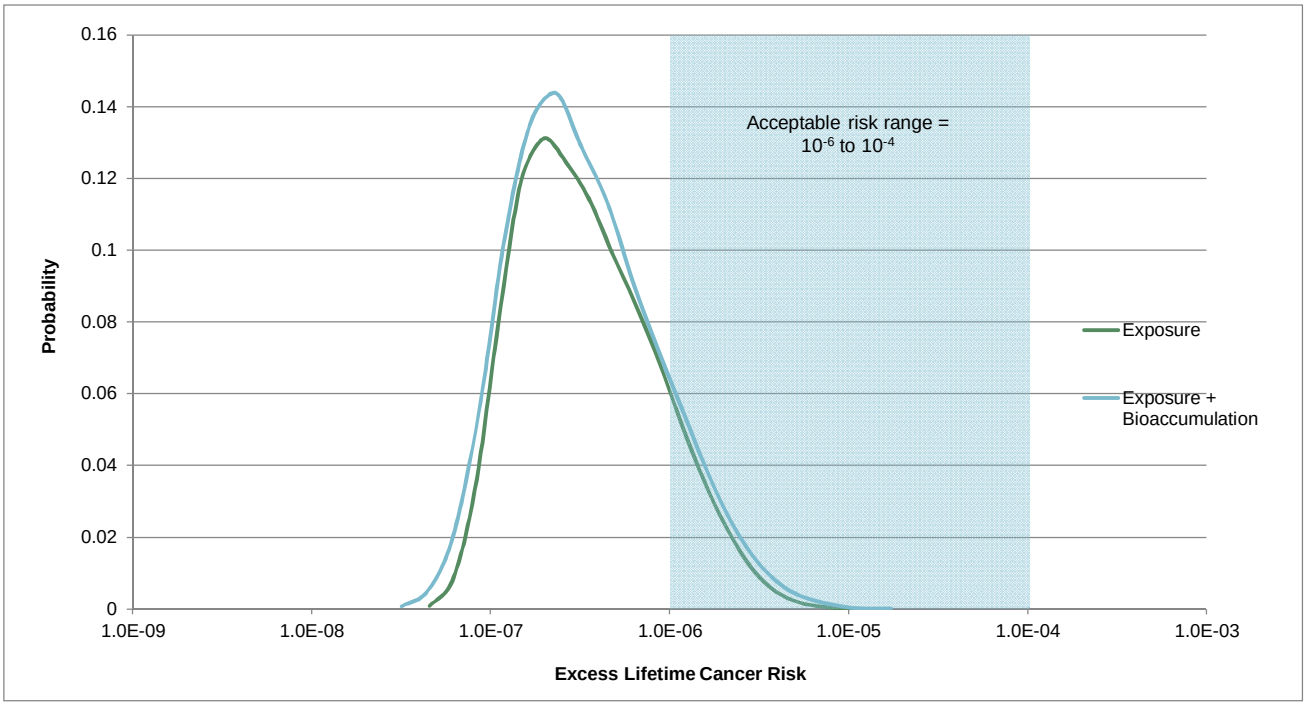
FIGURE 4



Distributions Used	Excess Lifetime Cancer Risk			
	Mean	Median	90th Percentile	95th Percentile
Exposure	4.6E-07	2.7E-07	1.0E-06	1.5E-06
Exposure + Bioaccumulation	4.7E-07	2.5E-07	1.1E-06	1.6E-06

PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

CASE STUDY: BENZO(A)PYRENE EXCESS LIFETIME CANCER RISK, VARIABILITY OF BIOACCUMULATION

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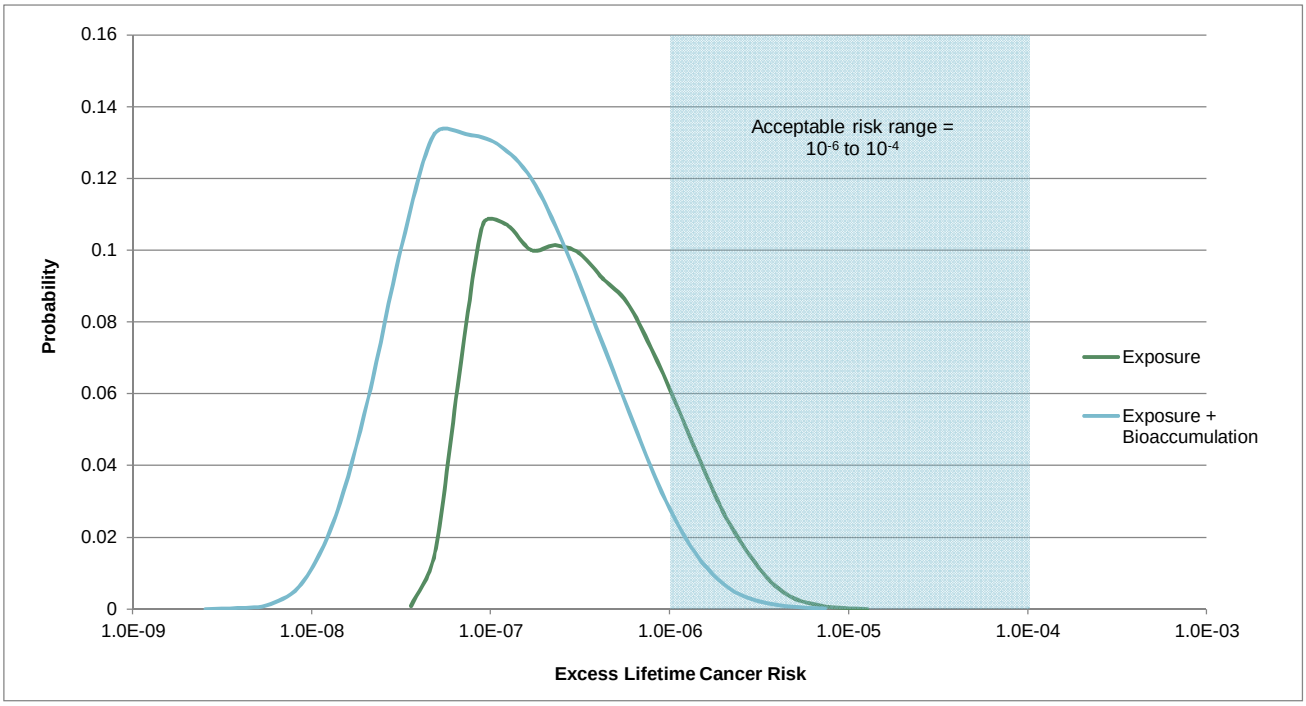
FIGURE 5



Distributions Used	Excess Lifetime Cancer Risk			
	Mean	Median	90th Percentile	95th Percentile
Exposure	4.4E-07	2.3E-07	1.1E-06	1.5E-06
Exposure + Bioaccumulation	1.8E-07	8.3E-08	4.2E-07	6.5E-07

PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

CASE STUDY: CHLORDANE LIFETIME CANCER RISK, VARIABILITY OF BIOACCUMULATION

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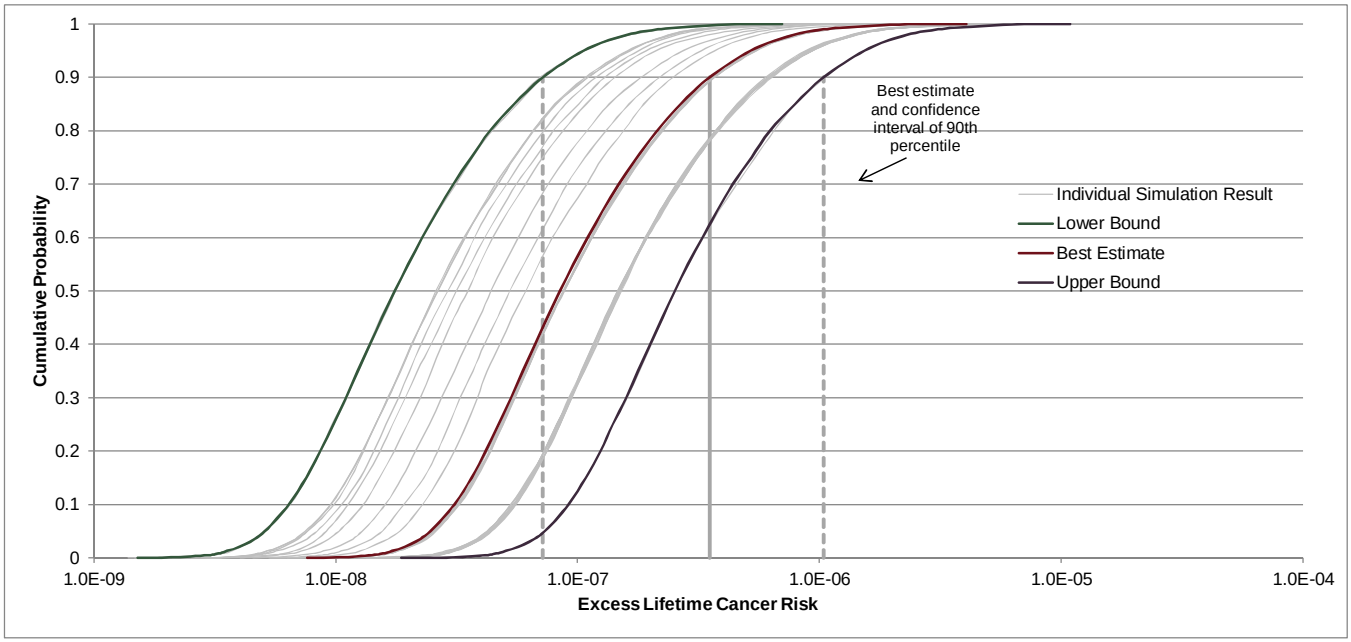
FIGURE 6



Percentile	Excess Lifetime Cancer Risk		
	Lower Bound (5th Percentile)	Best Estimate (Mean)	Upper Bound (95th Percentile)
50th Percentile	1.8E-08	8.5E-08	2.5E-07
90th Percentile	7.2E-08	3.5E-07	1.0E-06
95th Percentile	1.1E-07	5.2E-07	1.5E-06

PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

CASE STUDY: BENZO(A)PYRENE EXCESS LIFETIME CANCER RISK, UNCERTAINTY IN TOXICITY

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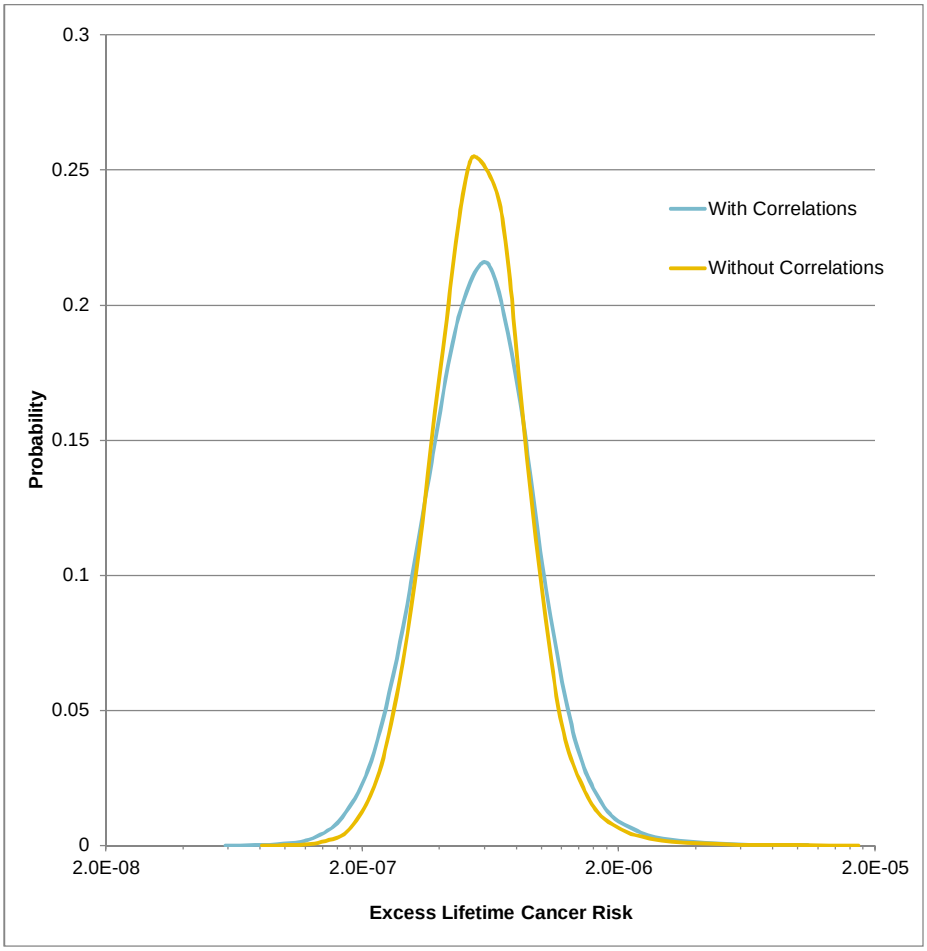
FIGURE 7



Percentile	Without Correlations [a]	With Correlations [b]
1%	1.6E-07	1.9E-07
5%	2.2E-07	2.5E-07
10%	2.7E-07	2.9E-07
15%	3.0E-07	3.3E-07
20%	3.3E-07	3.5E-07
25%	3.6E-07	3.8E-07
30%	3.9E-07	4.0E-07
35%	4.2E-07	4.3E-07
40%	4.5E-07	4.5E-07
45%	4.7E-07	4.8E-07
50%	5.0E-07	5.0E-07
55%	5.3E-07	5.3E-07
60%	5.7E-07	5.5E-07
65%	6.0E-07	5.8E-07
70%	6.4E-07	6.2E-07
75%	6.9E-07	6.5E-07
80%	7.5E-07	7.0E-07
85%	8.2E-07	7.6E-07
90%	9.2E-07	8.4E-07
95%	1.1E-06	1.0E-06
99%	1.8E-06	1.6E-06

Notes:

[a] No correlations defined between exposure parameters.

[b] Correlations defined between body weight and both drinking water intake and fish consumption rate.

PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

CORRELATIONS: BENZO(A)PYRENE EXCESS LIFETIME CANCER RISK

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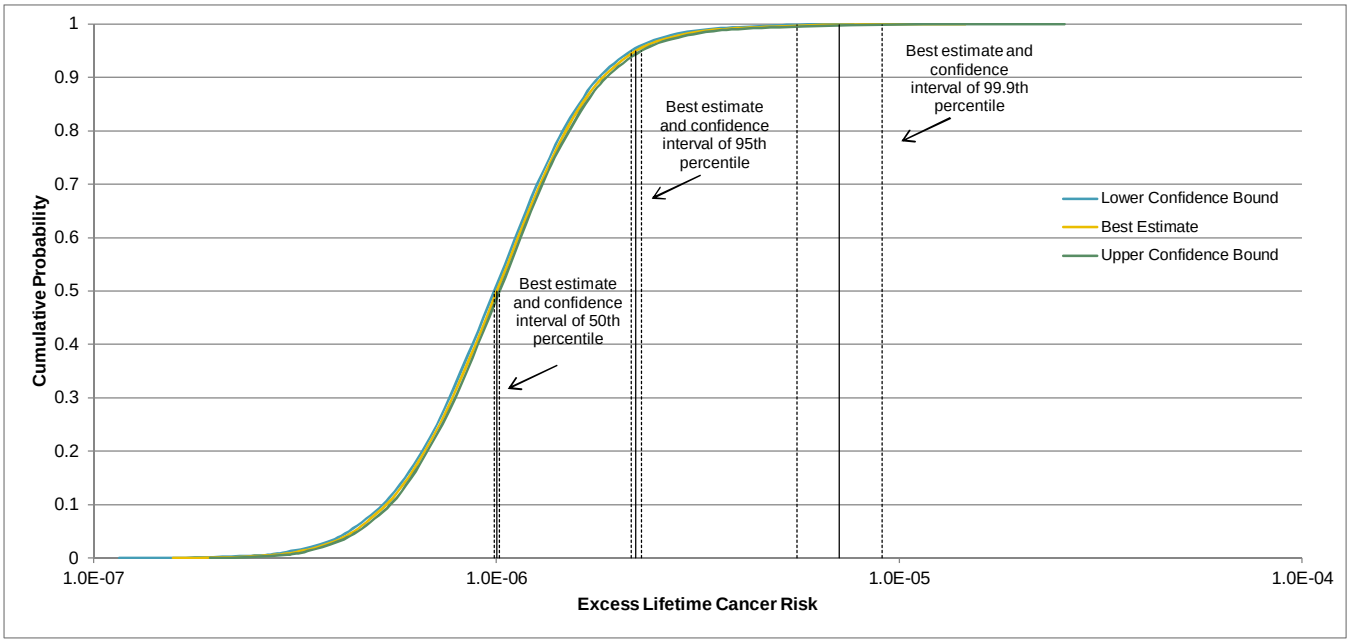
FIGURE 8



PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

EXTREME PERCENTILES: 2-DIMENSIONAL MONTE CARLO UNCERTAINTY ANALYSIS

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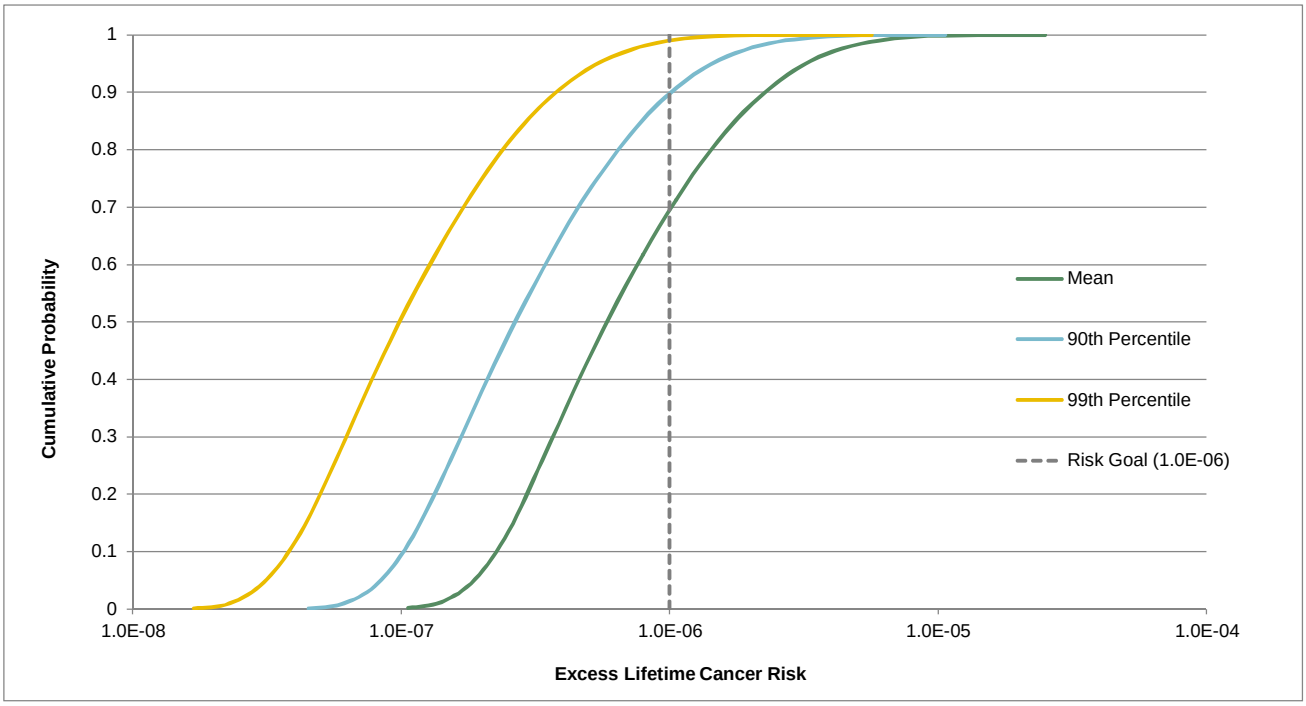
FIGURE 9



Population Percentile Targeted	BaP Criterion (ug/L)	Excess Lifetime Cancer Risk		
		Mean	90th Percentile	99th Percentile
Mean	0.0017	1.0E-06	2.2E-06	3.2E-06
90th	0.00076	4.5E-07	1.0E-06	2.7E-06
99th	0.00028	1.7E-07	3.8E-07	1.0E-06

PROBABILISTIC APPROACH TO DERIVING AMBIENT WATER QUALITY CRITERIA WHITE PAPER

HYPOTHETICAL AMBIENT WATER QUALITY CRITERIA DERIVED FOR BENZO(A)PYRENE

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FIGURE 10

ATTACHMENT K

Summary of Health Risk Assessment Decisions in Environmental Regulations

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Imagine the result

Northwest Pulp and Paper Association

Summary of Health Risk Assessment Decisions in Environmental Regulations

March 6, 2015

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Summary of Health Risk Assessment Decisions in Environmental Regulations

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Date:
March 6, 2015

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Table of Contents

Tables

Figures

Acronyms and Abbreviations

CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CWA	Clean Water Act
DBCP	dibromochloropropane
FFDCA	Federal Food, Drug and Cosmetic Act
g/day	grams per day
HHWQC	Human Health Water Quality Criteria
HQ	hazard quotient
LFC	lowest feasible concentration
LoREX	low release and exposure
MCL	Maximum Contaminant Level
MCLG	Maximum Contaminant Level Goal
mg/L	milligrams per liter
mg/yr	milligrams per year
MTCA	Model Toxics Control Act
NCEL	New Chemical Exposure Limit
NIOSH	National Institute of Occupational Safety and Health

NTP	National Toxicology Program
OSHA	Occupational Safety and Health Administration
PCB	polychlorinated biphenyls
PEL	Permissible Exposure Limit
REL	Recommended Exposure Limit
RfD	reference dose
SDWA	Safe Drinking Water Act
THM	trihalomethane
TSCA	Toxic Substances Control Act
TWA	time weighted average
USEPA	United States Environmental Protection Agency
USFDA	United States Food and Drug Administration

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Summary of Health Risk Assessment Decisions in Environmental Regulations

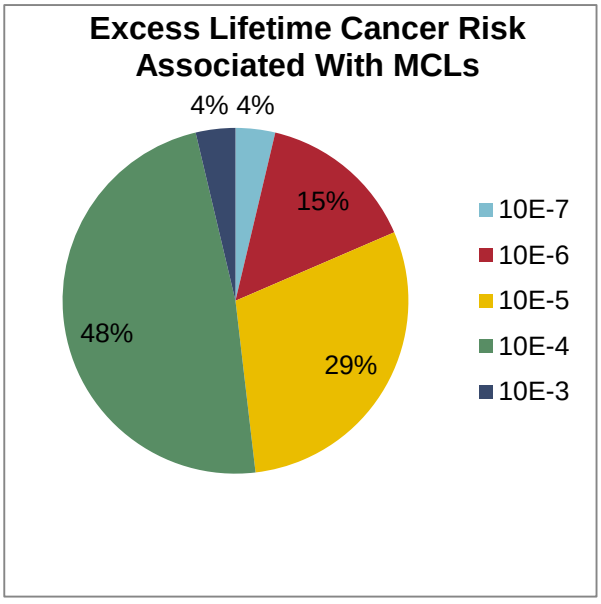
Executive Summary

This white paper provides perspective on how we protect human health through the choices reflected in environmental regulations. Limits on the concentrations of chemicals in the environment reflect a combination of science and policy. Regulators estimate the risks to human health from exposure to chemicals and then decide, as a matter of policy, what level of risk is acceptable. Those decisions are multi-faceted and reflect many smaller choices about both how to apply scientific knowledge and our values as a society. Wise choices must consider such decisions within the broader context of all the sources of risks to our health and the consequences of over-regulation.

Laying the groundwork: risk assessment concepts

Regulators estimate the potential risks to human health from exposure to chemicals in the environment by considering two factors: toxicity and exposure. The amount of a chemical to which people are exposed depends on how much of the chemical is in the air, water, soil, or food. It also depends on the amount of contact that people have with those media. The degree of contact – for example, the amount water that people drink or the amount of fish that people eat – can vary widely between people. Whether assessing the possible risks from environmental exposure or in setting limits on the acceptable concentrations in environmental media, regulators must decide what assumptions to make about the degree of exposure.

The risk of getting cancer from a lifetime of exposure to a chemical is expressed as a probability of developing cancer above and beyond the background risk that already exists, also known as the excess lifetime cancer risk. A $1x10^{-4}$ risk (or 1E-04) is a one in ten thousand chance of getting cancer over and above the background risk assuming a lifetime of exposure; a $1x10^{-6}$ risk (or 1E-06) is a one in a million chance. These risk levels represent the upper bound probability that an individual exposed to the chemical in the environment will develop cancer as a result of that exposure.



Putting risks into perspective

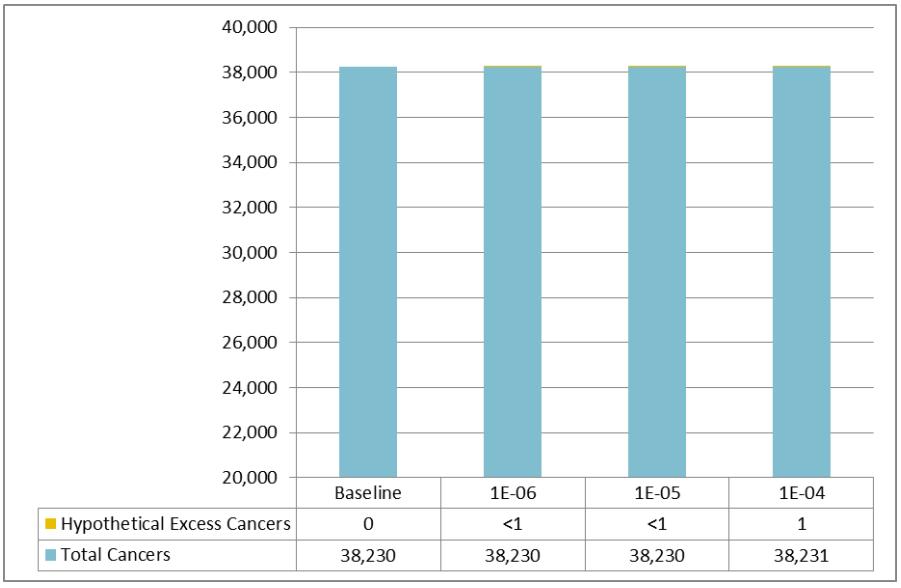
The debate over Human Health Water Quality Criteria (HHWQC) in Washington concerns in part the level of acceptable risk. This white paper discusses three factors that bear on this debate.

1. Acceptable risk from exposure to chemicals in the environment

Various statutes and associated regulations define acceptable risks differently. Standards set under the Occupational Safety and Health Act to protect workers on the job reflect an excess lifetime cancer risk on the order of $1x10^{-3}$. The limits on the concentrations of chemicals in our drinking water at the Maximum Contaminant Levels (MCLs) allowed reflect a range of excess lifetime cancer risks as depicted in the pie chart. Regarding HHWQC, the United States Environmental Protection Agency (USEPA) says this (USEPA 2000):

> *EPA also believes that criteria based on a 10^{-5} risk level are acceptable for the general population as long as States and authorized Tribes ensure that the risk to more highly exposed subgroups (sportfishers or subsistence fishers) does not exceed the 10^{-4} level.*

2. Comparison between risk of cancer from environmental exposure to regulated chemicals and risk of cancer from all causes



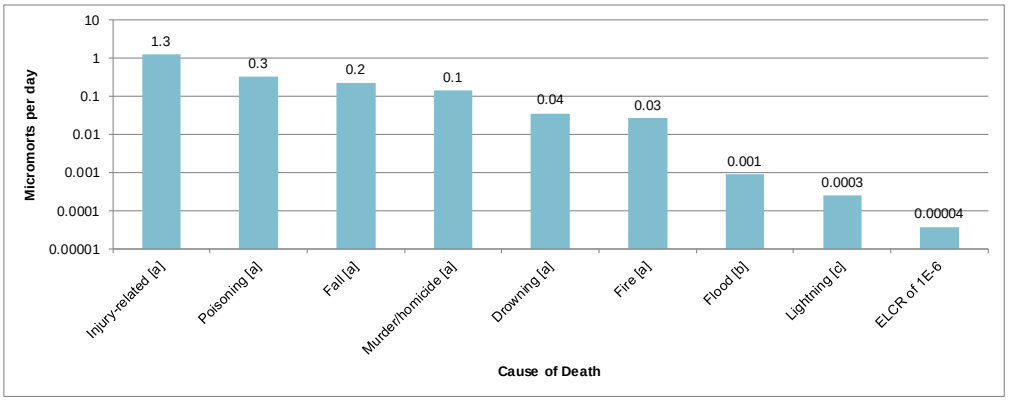
	Baseline	1E-06	1E-05	1E-04
Hypothetical Excess Cancers	0	<1	<1	1
Total Cancers	38,230	38,230	38,230	38,231

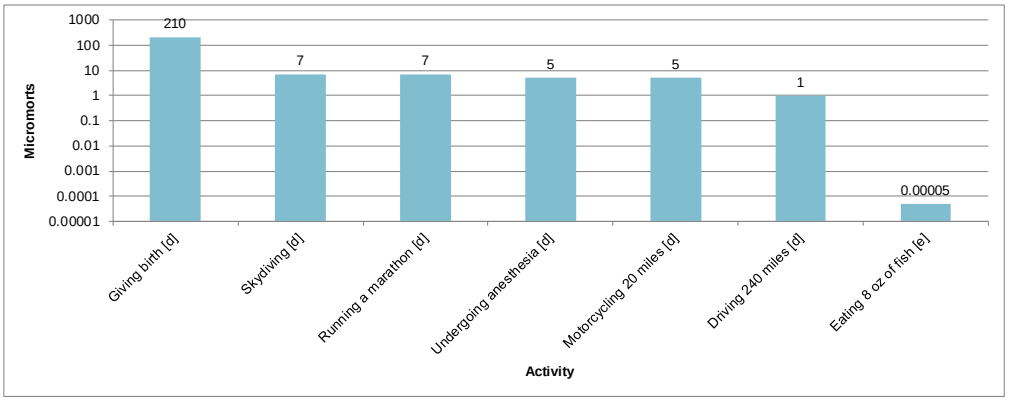
The risk of cancer from all causes far outweighs the possible risk of cancer from exposure to chemicals in the environment. The figure to the right shows how these risks translate to an estimated number of cancer occurrences per year in Washington State[1]. Compared to total cancer incidence in Washington, the increase in cancers associated with the excess lifetime cancer risks between $1x10^{-4}$ and $1x10^{-6}$ are far smaller (on the order of a thousandth of percent at an allowable excess lifetime cancer risk of $1x10^{-4}$ or less) than other causes of cancer. This finding is consistent with the comparisons of mortality risk associated with various allowable risk levels to mortality risk from various activities that are part of everyday life, as discussed below.

[1] Note that the in order to make the hypothetical excess cancers visible on the bar graph, the Y axis was set to start at 20,000 rather than 0.

3. Comparison between risk of cancer from environmental exposure and everyday risks

We face risks every day. When risk assessors want to be able to compare the relative risks from various activities they sometimes describe those risks in terms of “micromorts”. A micromort is an activity that typically occurs over time or distance which presents a risk of $1x10^{-6}$ (one in one million). As illustrated below, we routinely accept – whether we realize it or not – risks that far exceed an excess lifetime cancer risk of $1x10^{-4}$ to $1x10^{-6}$. The average American faced an unintentional injury-related mortality risk of approximately 467 micromorts per year in 2010, or 1.3 micromorts per day. In the U.S. population of 318 million people, the unit of 1.3 micromorts per day means that about 413 people die each day from an unintentional injury. This means that every day, every American has a risk of slightly greater than $1x10^{-6}$ of dying from unintentional injury. This every day, accepted risk provides context for discussions about protecting the general population and highly exposed subgroups.





Notes:

[a] Murphy et al. (2013)

[b] NOAA (2015a)

[c] NOAA (2015b)

[d] Blastland and Spiegelhalter (2014)

[e] Assuming organism-only AWQC are based on a fish consumption rate of 175 grams per day and risk level of $1x10^{-6}$.

Assumptions underlying risk characterization

Risk assessors must make many assumptions to estimate the possible risks from exposure to chemicals in the environment. These include assumptions about the degree of exposure. Assumptions about the amount of fish Washingtonians eat each day are particularly critical to the discussion about HHWQC though many other assumptions are important as well.

Water quality criteria based on the mean fish consumption rate in Washington and an excess lifetime cancer risk of $1x10^{-5}$ present a risk that, even to the most highly exposed populations, is within the acceptable range

as defined by USEPA (2000). The default fish consumption rate does not need to be raised to 175 grams per day to protect the people of Washington State from unreasonable risk. Why? Because conservative assumptions add up. If a decision maker chooses a conservative value for every variable in a risk calculation, the results will be far more protective than intended. Consider the hypothetical example of a risk assessment that is based on three independent and log-normally distributed parameters. In the case of a fish consumption calculation, those parameters might be the amount of fish eaten each day, the source of the fish, and the number of years over the course of a lifetime that people live in a certain place and eat fish from a local source. Each value represents the 95th percentile, or in other words that 9,500 out of 10,000 people have a lower exposure: they eat less fish, do not only eat fish from local waters, or do not eat local fish for their entire life, for example. Combining those three variables would result in a risk estimate that would fall at the 99.78th percentile of the resulting distribution. The risk to 9,978 out of 10,000 people would be lower than the allowable risk level used to establish the standard. So, if $1x10^{-5}$ was selected as the allowable risk level for a criterion based on those assumptions, 9,978 people would have a risk less than $1x10^{-5}$ and only 22 would have a risk greater than $1x10^{-5}$. Decisions made on the basis of this hypothetical calculation, which compounds conservative factors, are far more protective than intended if the goal was to protect the average member of the population (or the 90th percentile or even the 95th percentile of the population) at the selected allowable risk level.

This may look like an academic calculation. Some readers may think that overestimating risks is a good thing because it allows us to be extra-cautious, and that regulatory decisions based on risk estimates should be as conservative and protective as possible. But the consequences of such choices also need to be considered. There's a cost to reducing the levels of chemicals in the environment to meet more-stringent limits, a cost that may be measured in dollars, energy usage, or the risk of injury to workers who have the job of reducing the levels of those chemicals. Chemicals may be used to treat wastewater to meet lower standards, for example, and the sludge that results has to be trucked to a landfill or incinerated. Generating the power used to operate the wastewater treatment plant uses natural resources and creates air emissions. Each of these aspects of the life cycle of wastewater treatment operations, and their related risks, should be weighed against the value of regulatory decisions based on the combination of several conservative assumptions, referred to as compounded conservatism.

Compounding conservative values for multiple variables (including a high fish consumption rate, long duration of residence, and upper percentile drinking water rate) to estimate risks with a low target excess lifetime cancer risk will have an unintended consequence. It will result in HHWQC that are far more protective of the vast majority of the population than reflected by the target excess lifetime cancer risk. That additional degree of protection must be weighed against the risks and environmental impacts that would result from the additional treatment needed to meet such criteria.

1. Risk assessment concepts

This section provides some background information relevant to the topics discussed in this white paper. It begins with a general discussion of how both cancer and non-cancer risks are evaluated by the United States Environmental Protection Agency (USEPA) (Section 1.1). It then puts those risks into perspective by describing what risk assessment conclusions mean with respect to an individual or a larger group of people, and how cancers resulting from exposure to chemicals in the environment, if they occur, compare to the general incidence of cancer (Section 1.2).

1.1 Evaluation of cancer and noncancer health endpoints

Risk generally depends on the following factors (USEPA 2012A):

- Amount of exposure, which depends on
  - How much of a chemical is present in an environmental medium, such as soil, water, air, or fish;
  - How much contact (exposure) a person has with the environmental medium, containing the chemical; and
  - The toxicity of the chemical.

Scientists consider two types of toxic effects, cancer and noncancer, when they assess the possible risks to human health from exposure to chemicals in the environment. The ways in which most United States regulatory agencies evaluate these risks differ because of one fundamental assumption, that the human body can tolerate some low dose of a chemical that causes harm other than cancer but that no dose of a carcinogen (a chemical that may cause cancer) is entirely safe.

Chemicals that may cause cancer – or, in scientific terminology, those with a carcinogenic endpoint – are, with a very few exceptions, conservatively assumed to have some probability of causing an adverse health effect (cancer) at any dose, by typical regulatory risk assessment practice. There is no safe dose. Thus, *any* exposure to a chemical believed to cause cancer has associated with it a risk.

Carcinogenic risk is expressed as a probability of developing cancer as a result of a given level of exposure over a lifetime (USEPA 1989) above and beyond the background risk that already exists. This additional risk of getting cancer associated with exposure to chemicals is often referred to as the excess lifetime cancer risk. The excess lifetime cancer risk is usually described in scientific notation. A $1x10^{-4}$ risk (or 1E-04) is a one in ten thousand chance of getting cancer over and above the background risk assuming a lifetime of exposure; a $1x10^{-6}$ risk (or 1E-06) is a one in a million chance. These risk levels represent the upper bound probability that an individual exposed to the chemical in the environment will develop cancer as a result of that exposure. It's important to note that the probability pertains to the risk of getting cancer, not the risk of dying from cancer. These probabilities apply only to people who are exposed to the chemicals under the conditions and to the extent that was assumed in estimating the risk. (Typically, these risk levels correspond to 70 years of exposure and represent the risk over an entire lifetime.) It is also important to recognize that these are upper-bound estimates of risk that depend on numerous assumptions. The actual risks are expected to be lower and may be even be zero (USEPA 1986). Public health policy makers must choose some "acceptable" excess lifetime cancer risk (also referred to in this white paper as an allowable risk) when developing limits for chemicals in the environment.

Scientific Notation
One in a million is the same as…
1 in 1,000,000 or
1/1,000,000, or
0.000001, or
$1x10^{-6}$, or
1E-6, or
0.0001%

Chemicals that cause non-cancer adverse health effects are assumed to have some threshold dose below which no adverse health effects are expected to occur. In other words, test data show that there is a safe (or allowable) dose. Scientists use the hazard quotient (HQ) to indicate the degree of risk from exposure to a noncarcinogenic chemical:

HQ = (estimated exposure or dose) / (allowable dose).

An HQ of less than or equal to one indicates that the estimated exposure is less than or equal to the allowable dose (referred to by the USEPA as a reference dose or RfD) and that no adverse health effects are expected, even over a lifetime of continuous exposure. In other words, such exposures are considered safe. An HQ of greater than one indicates that estimated exposure is greater than the RfD. An exceedance of the RfD indicates that the potential exists for an adverse health effect to occur. However, because of the multiple conservative assumptions used to estimate exposures and to derive RfDs, an HQ somewhat greater than one is generally not considered to represent a substantial public health threat. The USEPA has offered this perspective (USEPA 1996):

> *Because many reference [doses] incorporate protective assumptions designed to provide a margin of safety, a hazard quotient greater than one does not necessarily suggest a likelihood of adverse effects. A hazard quotient less than one, however, suggests that exposures are likely to be without an*

> *appreciable risk of noncancer effects during a lifetime. Furthermore, the hazard quotient cannot be translated into a probability that an adverse effects [sic] will occur, and is not likely to be proportional to risk. A hazard quotient greater than one can be best described as only indicating that a potential may exist for adverse health effects.*

The United States Department of Health and Human Services (2013) provides further perspective:

> *If the hazard quotient exceeds unity, the toxicant may produce an adverse effect but normally this will require a hazard quotient of several times unity; a hazard quotient of less than one indicates that no adverse effects are likely over a lifetime of exposure.*

In short, while an HQ less than one provides substantial certainty that exposure will not result in a risk, exposure that results in an HQ of somewhat greater than one (even up to several times one) is also unlikely to result in an adverse effect.

1.2 Perspective on cancer risks

The excess lifetime cancer risk that may occur as a result of exposure to a carcinogen in the environment, as described above, is the excess risk above and beyond the background risks that we all face. The American Cancer Society provides perspective on background risks. It estimates that in 2014, 1,665,540 new cancer cases were diagnosed in the United States and 585,720 people died of cancer. These numbers include 38,230 new diagnoses and 12,550 deaths in the state of Washington. **Table 1** summarizes the incidence of cancer in the United States and in the state of Washington in 2014.

Table 1 Incidence of Cancer in 2014, from all causes

Geography	Cancer Cases Diagnosed in 2014*	Estimated Population in 2014**	Annual Cancer Incidence Rate
U.S. (national)	1,665,540	318,857,056	5.22×10^{-3}
Washington State	38,230	7,061,530	5.41×10^{-3}

* American Cancer Society 2014.

** U.S. Census Bureau 2014.

As the data in Table 1 show, a person living in the United States has about a 5/1,000 chance, *per year*, equal to about a 3.7 in 10 chance (37%) over a 70-year lifetime, of being diagnosed with cancer. In contrast, many regulatory agencies believe that an "acceptable" excess lifetime cancer risk that should be used to set limits on chemicals in the environment should correspond to a risk of 1/10,000 (1×10^{-4}) to 1/1,000,000 (1×10^{-6}) over the course of a *lifetime*. **Table 2** shows how the annual risk of cancer from all causes, based on the 2014 data shown in Table 1, compares to the annual cancer risk that would result from exposure to

compounds in the environment that met environmental standards based on a lifetime cancer risk of $1x10^{-4}$ to $1x10^{-6}$. The cancer risk from exposures to environmental pollutants at or below their environmental standards is a tiny fraction (0.028% to 0.00028%) of the background cancer risk we all face.

Table 2 Incidence of Cancer in 2014 Compared to Acceptable Risk under Environmental Regulations

Geography	Annual Cancer Incidence Rate based on 2014 Data	Annual Risk of Cancer associated with Lifetime Excess Lifetime Cancer Risk $1x10^{-4}$	Annual Risk of Cancer associated with Lifetime Excess Lifetime Cancer Risk $1x10^{-6}$
United States (national)	$5.2x10^{-3}$ (0.52%)	$1.4x10^{-6}$ (0.00014%)	$1.4x10^{-8}$ (0.0000014%)
Washington State	$5.4x10^{-3}$ (0.54%)	$1.4x10^{-6}$ (0.00014%)	$1.4x10^{-8}$ (0.0000014%)

2. Risk assessment choices in federal regulatory programs

We've been assessing the risks from exposure to chemicals in the United States for just over half a century. In 1958, scientists knew of just four human carcinogens; by 1978, they knew of 37 human carcinogens and over 500 animal carcinogens (Wilson 1978). The National Toxicology Program (NTP) currently lists 243 agents, substances, mixtures, and exposure circumstances that *are* known or reasonably anticipated *to* cause cancer in humans (NTP 2014). Environmental legislation that developed in the United States in parallel to the study of what could cause cancer reflected both our scientific understanding of the hazards of chemical exposure and the socioeconomic factors of the times. Much of the legislation requiring assessment of risks of exposure to chemicals in the environment originated between 1972 and 1980[2].

This perspective is important when considering the risk assessment choices expressed in federal regulatory programs. Congress and regulators had to articulate their thinking about risk and what levels of risk were acceptable over a relatively short period of time. We had little time to test and debate ideas, as a society, about how what levels of risk are acceptable to us. It is useful, then, to take the "big picture" view of acceptable risk as we discuss risk based water quality criteria in Washington State.

Various federal laws and regulations define 'acceptable risk' in different ways. These definitions typically fall into one or more of the general categories shown in **Table 3** (Schroeder 1990).

[2] Includes: Clean Water Act (1972), Clean Air Act (1972), Safe Drinking Water Act (1974), Resource Conservation and Recovery Act (1976), Comprehensive Environmental Response, Compensation, and Liability Act (1980).

Table 3 Ways of Reflecting Risk Considerations in Environmental Laws

Type of standard	Variation	Premise
Health based standards	Zero risk	Risk should be reduced to zero or to some other level that is acceptable to society
	Significant risk	
Balancing standards	Cost-benefit	Possible risks must be balanced against the economic benefits of using a chemical or the costs of controlling risks
Technology based standards	Feasibility analysis	Limits are set based on the levels achievable by the best available treatment technology that the regulated industry can afford to install.

As a result of the different ways of thinking about acceptable risk and the factors that must be taken into account when regulating exposure to chemicals, regulators have defined goals for limiting cancer risks in different ways in various regulatory programs. **Table 4** summarizes benchmark criteria. Those criteria and some of the striking differences between programs are described below.

Table 4 Benchmarks for "Acceptable" Risk

Law / Regulation	Focus	Risk Standard	Criterion for Carcinogens
Clean Water Act	Surface water	Adverse health impacts	$1x10^{-4}$ to $1x10^{-6}$
Safe Drinking Water Act	Public drinking water	Any adverse effect	Goal: 0 Enforceable standard: $1x10^{-4}$ to $1x10^{-7}$
Toxic Substances Control Act	Chemicals manufactured or imported into the United States	Unreasonable risk	$1x10^{-4}$ (inferred, absent clear policy)
Occupational Safety and Health Act	Worker protection	Significant risk over 45-year working life	$1x10^{-3}$
Comprehensive Environmental Response, Compensation, and Liability Act, or Superfund	Uncontrolled hazardous waste sites	No significant risk	$1x10^{-4}$ to $1x10^{-6}$

2.1 The beginning of "minimal risk" discussions: the Delaney Clause

Delaney Clause – 1958
- Health based standards ✓
- Balancing standards
- Technology based standards

The debate over what level of exposure to a carcinogen could be considered safe began in the United States when people became concerned about pesticide residues in processed foods. This debate produced the 1958 Food Additives Amendment (section 409) to the 1954 Federal Food, Drug and Cosmetic Act (FFDCA), which said:

> *…no additive shall be deemed to be safe if it is found to induce cancer when ingested by man or animal, or if it is found, after tests which are appropriate for the evaluation of the safety of food additives, to induce cancer in man or animal…*

This "zero risk" clause, named for Congressman James Delaney, was a landmark decision in the regulation of compounds that might cause cancer. The Delaney Clause sounds simple enough, but soon ran into practical limitations: How low of a dose do we need to test to assure ourselves that a chemical does not cause cancer? And how, given the limits of analytical chemistry, do we know when a chemical that can induce cancer is present in a food product?

The United States Food and Drug Administration (USFDA) faced this challenge in regulations proposed in 1973 (USFDA 1973), saying:

> *If the results of the test for carcinogenicity establish that the compound or its metabolites will induce cancer in test animals, the required sensitivity of the regulatory assay method will be determined based on the Mantel-Bryan procedure ….*
>
> *Absolute safety can never be conclusively demonstrated experimentally. The level defined by the Mantel-Bryan procedure is an arbitrary but conservative level of maximum exposure resulting in a minimal probability of risk to an individual (e.g., 1/100,000,000), under those exposure conditions of the basic animal studies.*

In describing the benchmark (1/100,000,000 or 10^{-8}) provided as an example of minimal probability of risk to an individual, the USFDA cited a groundbreaking paper by Mantel and Bryan (1961) that said:

> *We may, for example, assume that a risk of 1/100 million is so low as to constitute "virtual safety." Other arbitrary definitions of "virtual safety" may be employed as conditions require.*

Many of the comments on the regulation proposed in 1973 pertained to how the proposed regulation dealt with the risk of cancer and the 1/100,000,000 benchmark. After considering those comments the USFDA promulgated a final regulation in 1977. In doing so it re-defined the benchmark risk level. The preamble to

the final rule explains that tests for carcinogens must be able to measure the concentration corresponding to the 1/1,000,000 (or 10^{-6}) risk level, which the USFDA described as an "insignificant public health concern". (USFDA 1977)

In this rulemaking, the USFDA was careful to point out that it was not making an explicit judgment on an acceptable level of risk, simply seeking to set a practical benchmark that could be used to design animal experiments:

> *[10^{-6}] does not represent a level of residues "approved" for introduction into the human diet. The purpose of these regulations is to establish criteria for the evaluation of assays for the measurement of carcinogenic animal drugs. These criteria must include some lowest level of reliable measurement that an assay is required to meet. In defining a level of potential residues that can be considered "safe", therefore, the Commissioner is establishing a criterion of assay measurement that, if it can be met for a compound, will ensure that any undetected residues resulting from the compound's use will not increase the risk of human cancer.*

Despite this caution, many people took this regulatory action as a precedent for defining an "acceptable" level of risk as $1x10^{-6}$. In fact, the Delaney Clause was replaced in 1996 by legislation that specifies 10^{-6} as an acceptable level of risk[3] (Moran 1977).

2.2 Clean Water Act

Under the Clean Water Act (CWA), States and authorized Native American tribes set water quality standards for the surface water bodies under their jurisdiction. A water quality standard has two parts: the designated uses of a body of water, and the criteria (or concentration limits for specific chemical compounds) necessary to protect those uses. The USEPA develops Human Health Water Quality

CWA – 1972	
Health based standards	✓
Balancing standards	
Technology based standards	

[3] The Delaney Clause is no longer in effect. The Food Quality Protection Act of 1996 changed the standard for the residues of carcinogens in foods from the "zero risk" criterion implicit in the Delaney Clause to a standard of "reasonable certainty that no harm will result from aggregate exposure to the pesticide chemical residue." The law allows for chemical residues if the risk of causing cancer in less than one-in-a-million people over the course of a typical life-span. The USEPA must consider the benefits of pesticides in supporting an adequate, wholesome, and economical food supply in determining an acceptable level of risk.

Criteria (HHWQC) that States and Native American tribes can use to set those concentration limits (USEPA 2000). In general (USEPA 2000),

> *Water quality criteria are derived to establish ambient concentrations of pollutants which, if not exceeded, will protect the general population from adverse health impacts from those pollutants due to consumption of aquatic organisms and water, including incidental water consumption related to recreational activities.*

For compounds that may cause cancer in people exposed to surface water, those criteria must correspond to some level of risk that is thought to be acceptable.

The USEPA's 1980 HHWQC National Guidelines simply represented a range of risks. In other words, the guidance presented a range of chemical concentrations corresponding to incremental cancer risks of 10^{-7} to 10^{-5}. Revised guidelines published in 2000 corresponded to the 10^{-6} risk level, with this explanation (USEPA 2000):

> *With [HHWQC] derived for carcinogens based on a linear low-dose extrapolation, the Agency will publish recommended criteria values at a 10^{-6} risk level. States and authorized Tribes can always choose a more stringent risk level, such as 10^{-7}. EPA also believes that criteria based on a 10^{-5} risk level are acceptable for the general population as long as States and authorized Tribes ensure that the risk to more highly exposed subgroups (sportfishers or subsistence fishers) does not exceed the 10^{-4} level.*

The Agency elaborated on this policy with respect to more highly exposed people, saying

> *EPA understands that highly exposed populations may be widely distributed geographically throughout a given State or Tribal area. EPA recommends that priority be given to identifying and adequately protecting the most highly exposed population. Thus, if the State or Tribe determines that a highly exposed population is at greater risk and would not be adequately protected by criteria based on the general population, and by the national … criteria in particular, EPA recommends that the State or Tribe adopt more stringent criteria using alternative exposure assumptions….*
>
> *EPA understands that fish consumption rates vary considerably, especially among subsistence populations, and it is such great variation among these population groups that may make either 10^{-6} or 10^{-5} protective of those groups at a 10^{-4} risk level. Therefore, depending on the consumption patterns in a given State or Tribal jurisdiction, a 10^{-6} or 10^{-5} risk level could be appropriate. In cases where fish consumption among highly exposed population groups is of a magnitude that a 10^{-4} risk level would be exceeded, a more protective risk level should be chosen.*

> *…changing the exposure parameters also changes the risk. Specifically, the incremental cancer risk levels are relative, meaning that any given criterion associated with a particular cancer risk level is also associated with specific exposure parameter assumptions (e.g., intake rates, body weights). When these exposure parameter values change, so does the relative risk. For a criterion derived on the basis of a cancer risk level of 10^{-6}, individuals consuming up to 10 times the assumed fish intake rate would not exceed a 10^{-5} risk level. Similarly, individuals consuming up to 100 times the assumed rate would not exceed a 10^{-4} risk level. Thus, for a criterion based on EPA's default fish intake rate (17.5 gm/day) and a risk level of 10^{-6}, those consuming a pound per day (i.e., 454 grams/day) would potentially experience between a 10^{-5} and a 10^{-4} risk level (closer to a 10^{-5} risk level).*

In other words, the USEPA generally sets HHWQC at the 10^{-5} to 10^{-6} risk level, but allows states and tribes flexibility in setting enforceable criteria. In regions where some groups may eat more fish than is typical and by doing so perhaps increase their exposure to chemicals in fish, the Agency advises that the criterion set for the general population should not result in a risk to those who eat more fish that is greater than 10^{-4}.

2.3 Safe Drinking Water Act

The USEPA sets two kinds of criteria for chemicals in public water supplies, Maximum Contaminant Level Goals (MCLGs) and Maximum Contaminant Levels (MCLs). Here's how the Agency describes the process of determining those criteria (USEPA 2013A):

> *If there is evidence that a chemical may cause cancer, and there is no dose below which the chemical is considered safe, the MCLG is set at zero. If a chemical is carcinogenic and a safe dose can be determined, the MCLG is set at a level above zero that is safe….*
>
> *Once the MCLG is determined, EPA sets an enforceable standard. In most cases, the standard is a Maximum Contaminant Level (MCL), the maximum permissible level of a contaminant in water which is delivered to any user of a public water system. …The MCL is set as close to the MCLG as feasible….. EPA may adjust the MCL for a particular class or group of systems to a level that maximizes health risk reduction benefits at a cost that is justified by the benefits.*

The USEPA also determines non-enforceable Drinking Water Specific Risk Level Concentrations. It has described the Drinking Water Specific Risk Level Concentration as being based on the $1x10^{-4}$ excess lifetime cancer risk (USEPA 2012B). In some cases, as illustrated in **Table 5**, adjustments to the MCL have resulted in a concentration limit that corresponds to a higher risk. In other cases, the MCL for a chemical is lower than the concentration corresponding to the 10^{-4} risk level and therefore represents a lower risk level.

SDWA – 1972	
Health based standards	✓
Balancing standards	✓
Technology based standards	✓

Table 5 Comparison of Drinking Water MCLs and Cancer Risk Levels for Potential Carcinogens

Compound	MCL* (mg/L)	Concentration (mg/L) at 10^{-4} Cancer Risk*	Approximate Risk Level of MCL
Arsenic	0.01	0.002	$5x10^{-4}$
Benzene	0.005	1 to 10	$5x10^{-7}$ to $5x10^{-6}$
Benzo(a)pyrene	0.0002	0.0005	$4x10^{-5}$
Bromodichloromethane (THM**)	0.1	0.08	10^{-4}
Bromate	0.01	0.005	$2x10^{-4}$
Bromoform (THM**)	0.08	0.08	10^{-4}
Carbon tetrachloride	0.005	0.05	10^{-5}
Chlordane	0.002	0.01	$2x10^{-5}$
Di(2-ethylhexyl)adipate	0.4	3	10^{-5}
Dibromochloromethane (THM**)	0.08	0.08	10^{-4}
Dibromochloropropane (DBCP)	0.0002	0.003	$7x10^{-6}$
Dichloroacetic acid+	0.06	0.07	10^{-4}
Dichloroethane (1,2-)	0.005	0.04	10^{-5}
Dichloroethylene (1,1-)	0.007	0.006	10^{-4}
Dichloromethane	0.005	0.5	10^{-6}
Dichloropropane (1,2-)	0.005	0.06	10^{-5}
Epichlorohydrin	TT++	0.3	$7x10^{-7}$
Ethylene dibromide	0.00005	0.002	$2.5x10^{-6}$
Heptachlor	0.0004	0.0008	$5x10^{-5}$
Heptachlor epoxide	0.0002	0.0004	$5x10^{-5}$
Hexachlorobenzene	0.001	0.002	$5x10^{-5}$
Pentachlorophenol	0.001	0.009	10^{-5}
Polychlorinated biphenyls (PCBs)	0.005	0.01	$5x10^{-5}$
2,3,7,8-TCDD (dioxin)	$3x10^{-8}$	$2x10^{-8}$	10^{-4}
Toxaphene	0.003	0.003	10^{-4}
Trichloroethylene	0.005	0.3	10^{-6}
Vinyl chloride	0.002	0.002	10^{-4}

* USEPA 2012B.

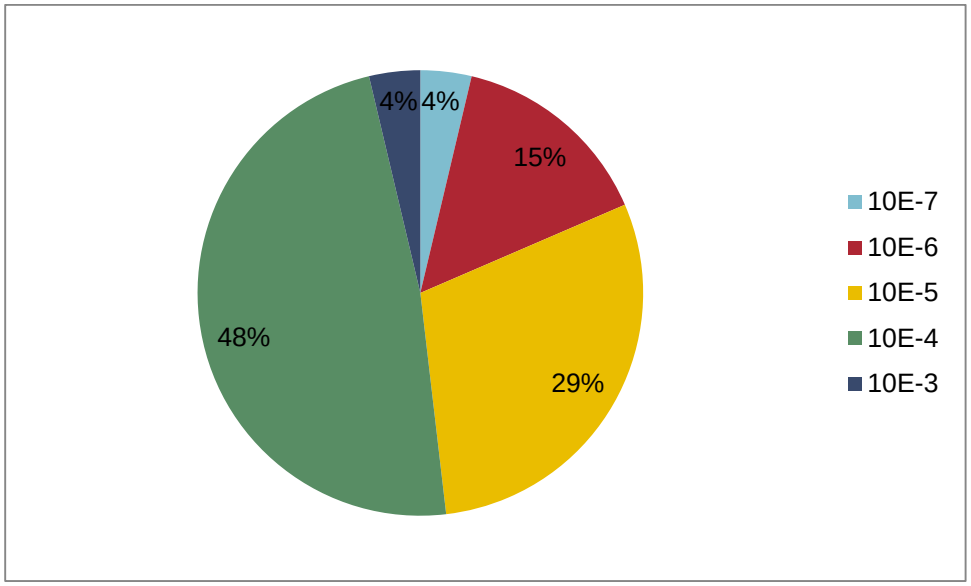
** Total trihalomethane (THM) concentration should not exceed 0.08 mg/L.

+ The total for five haloacetic acids is 0.06.

++ When epichlorohydrin is used in drinking water systems, the combination (or product) of dose and monomer level shall not exceed that equivalent to an epichlorohydrin-based polymer containing 0.01% monomer dosed at 20 mg/L. (0.01/100 * 20 mg/L = 0.002 mg/L)

As these examples show and as illustrated in **Figure 1**, the excess lifetime cancer risks associated with a single drinking water contaminant present in a water supply at its MCL may fall within a range of several orders of magnitude. Forty-eight percent of MCLs correspond to an estimated lifetime risk of $1x10^{-4}$ to $1x10^{-3}$; 29% of MCLs represent a potential risk of cancer after a lifetime of exposure of $1x10^{-5}$ to $1x10^{-4}$. While the USEPA may consider the benchmark excess lifetime cancer risk of 10^{-4} in setting a standard, the requirement to set the MCL as close to the MCLG as feasible or to adjust the MCL to a level that "maximizes health risk reduction benefits at a cost that is justified by the benefits" may result in a MCL that represents a very different risk level for that compound. And the combined risks of exposure to multiple chemicals, if they are present in the water supply, may increase the potential risk further.

Figure 1 Approximate Risk Levels associated with MCLs in Drinking Water



2.4 Occupational Safety and Health Act

The United States Occupational Safety and Health Administration (OSHA) develops standards to protect workers under the Occupational Safety and Health Act of 1970. OSHA first promulgated standards in 1974 to regulate the industrial use of 13 chemicals identified as potential occupational carcinogens. Those standards did not set limits on exposure, simply mandated the use of engineering controls, work practices, and personal protective equipment to limit exposure.

OSHA has since promulgated standards for certain carcinogens, including the regulations at 1910 Subpart Z, Toxic and Hazardous Substances. Those standards reflect a landmark decision by the Supreme Court known as the “Benzene Decision”, more formally known as *Industrial Union Department v. American*

Petroleum Institute, 448 U.S. 607, in 1980, At issue was whether setting worker protection standards for carcinogens such as benzene at the lowest technologically feasible level that would not impair the viability of the industries regulated conformed to the statutory requirement that such standards be "reasonably necessary or appropriate to provide safe and healthful employment". The decision read, in part,

> *… "safe" is not the equivalent of "risk-free." A workplace can hardly be considered "unsafe" unless it threatens the workers with a significant risk of harm…. [T]he requirement that a "significant" risk be identified is not a mathematical straitjacket. It is the Agency's responsibility to determine, in the first instance, what it considers to be a "significant" risk. Some risks are plainly acceptable and others are plainly unacceptable. If, for example, the odds are one in a billion that a person will die from cancer by taking a drink of chlorinated water, the risk clearly could not be considered significant. On the other hand, if the odds are one in a thousand that regular inhalation of gasoline vapors that are 2% benzene will be fatal, a reasonable person might well consider the risk significant and take appropriate steps to decrease or eliminate it. Although the Agency has no duty to calculate the exact probability of harm, it does have an obligation to find that a significant risk is present before it can characterize a place of employment as "unsafe."*

The Supreme Court essentially stated that a risk of fatality of 1×10^{-3} in an occupational setting was unacceptable. OSHA applied this benchmark to excess lifetime cancer risk. (Again, it is worth noting that not all cancers are fatal: an excess lifetime cancer risk of 1×10^{-3} corresponds to a far lower risk of cancer-related death.) For example, when OSHA set the Permissible Exposure Limit (PEL) for methylene chloride as a time weighted average (TWA) concentration, it offered an explanation that indicated how it thought about acceptable risk and acknowledged the level of risk associated with the standard being replaced (OSHA 1997):

> *OSHA's final estimate of excess cancer risks at the current PEL of 500 [parts per million] ppm (8-hour TWA) is 126 per 1000. The risk at the new PEL of 25 ppm is 3.62 per 1000. The risk at 25 ppm is similar to the risk estimated in OSHA's preliminary quantitative risk assessment based on applied dose of [methylene chloride] on a mg/kg/day basis (2.3 per 1000 workers) and clearly supports a PEL of 25 ppm. Risks greater than or equal to 10(-3) are clearly significant and the Agency deems them unacceptably high. However, OSHA did not collect the data necessary to document the feasibility of a PEL below 25 ppm across all affected industry sectors, and so the Agency has set the PEL at 25 ppm in the final rule.*
>
> *Further guidance for the Agency in evaluating significant risk and narrowing the million-fold range provided in the "Benzene decision" is provided by an examination of occupational risk rates, legislative intent, and the academic literature on "acceptable risk" issues. For example, in the high risk occupations of mining and quarrying, the average risk of death from an occupational injury or an acute occupationally-related illness over a lifetime of employment (45 years) is 15.1 per 1,000*

> *workers. The typical occupational risk of deaths for all manufacturing industries is 1.98 per 1,000. Typical lifetime occupational risk of death in an occupation of relatively low risk, like retail trade, is 0.82 per 1,000. (These rates are averages derived from 1984-1986 Bureau of Labor Statistics data for employers with 11 or more employees, adjusted to 45 years of employment, for 50 weeks per year).*

The National Institute of Occupational Safety and Health, or NIOSH, is the research and development counterpart to OSHA. Part of the organization's mission is to develop recommendations for health and safety standards. Their work provides guidance on limits for occupational exposures that supplements and informs OSHA rulemaking.

In 1976, NIOSH published its first guidelines on carcinogens in the workplace. Those guidelines called for "no detectable exposure levels for proven carcinogenic substances" (NIOSH 2014). NIOSH set Recommended Exposure Limits (RELs) for most carcinogens at the "lowest feasible concentration (LFC)." In 1995, NIOSH revised its policy (NIOSH 2010):

> *NIOSH recommended exposure limits (RELs) will be based on risk evaluations using human or animal health effects data, and on an assessment of what levels can be feasibly achieved by engineering controls and measured by analytical techniques. To the extent feasible, NIOSH will project not only a no-effect exposure, but also exposure levels at which there may be residual risks.*
>
> *The effect of this new policy will be the development, whenever possible, of quantitative RELs that are based on human and/or animal data, as well as on the consideration of technological feasibility for controlling workplace exposures to the REL..*

In 2013, NIOSH issued a new carcinogen policy for public comment. This policy explicitly addresses the acceptable level of risk from exposure to carcinogens in the workplace. In a document titled *NIOSH Current Intelligence Bulletin: Update of NIOSH Carcinogen Classification and Target Risk Level Policy for Chemical Hazards in the Workplace*, NIOSH proposed the following (NIOSH 2013).

> *NIOSH will set RELs to keep exposures below the 95% lower confidence limit estimate of the dose expected to produce 1 in 1,000 excess risk of cancer as a result of a 45-year working lifetime exposure (section 6). Although NIOSH recommends keeping occupational carcinogen exposures below the concentrations that produce a working lifetime risk of 1 in 1,000, this should be considered the minimum level of protection. Controlling exposures to lessen risk is always warranted….*
>
> *The 1 in 1,000 risk level comes from interpreting the 1980 U.S. Supreme Court "benzene" decision, which determined a 1 in 1,000 excess risk to be significant.*

In summary, the levels of risk considered to be acceptable for workers have varied over time at OSHA and at NIOSH. In the latest evolution of policy, an excess risk of 1/1000 ($1x10^{-3}$) over a working lifetime of 45 years of exposure has been proposed as the basis for workplace standards, although some standards, former and current, have exceeded that limit. By comparison to the other definitions of acceptable risk described in this white paper, this risk equates to an annual risk of $2x10^{-5}$ or an excess lifetime cancer risk (70 years) of approximately $2x10^{-3}$.

2.5 Toxic Substances Control Act

The Toxic Substances Control Act, abbreviated TSCA, regulates most chemical substances manufactured or imported into the United States. Under this law the USEPA can require reporting, record-keeping and testing of chemical substances, and may impose restrictions on their manufacture or use. The law defines the conditions under which the USEPA can take action. If an "unreasonable risk of injury to health or the environment" from a chemical substance has been proven, for example, the Agency can require risk-abatement action such as labeling chemical substances, regulating uses, restrictions on disposal, and prohibiting or limiting manufacture. But neither the law nor the regulations that implement the law define "unreasonable risk" clearly.

The USEPA has not published explicit guidance on how it reaches a finding of "unreasonable risk" but has described it generally as follows (USEPA 2013B):

> *EPA's determination that manufacture, processing, use, distribution in commerce, or disposal of an individual substance which has been the subject of a notice under section 5 of the TSCA may present an unreasonable risk of injury to human health or the environment is based on consideration of (i) the size of the risks identified by EPA; (ii) limitations on risk that would result from specific safeguards (generally, exposure and release controls) sought based on Agency review and (iii) the benefits to industry and the public expected to be provided by new chemical substances intended to be manufactured after Agency review. In considering risk, EPA considers factors including environmental effects, distribution, and fate of the chemical substance in the environment, disposal methods, waste water treatment, use of protective equipment and engineering controls, use patterns, and market potential of the chemical substance.*

What does this mean with respect to the acceptable level of cancer risk for workers manufacturing a new chemical or consumers who might be exposed to it? The USEPA has not published a clear statement on acceptable risk under TSCA, but the cases described

TSCA – 1976	
Health based standards	✓
Balancing standards	✓
Technology based standards	✓

below shed some light on the question[4]. The first is a publication by an Agency official early in the TSCA program regarding the determination of acceptable risks under TSCA, and the second, the USEPA's explanation of how it derives limits for worker exposure to new chemicals under TSCA.

In 1983, a USEPA official indicated that the objective is to reduce risks to an "insignificant" level but that the USEPA did "not employ any predetermined statistical risk level since this will vary depending on a variety of factors." (Todhunter 1983). In other words, at that time "unreasonable risk" did not correspond to a benchmark level or range (such as 10^{-4} to 10^{-6}). The USEPA has not apparently published anything since that time to suggest that a benchmark level exists under TSCA, with one exception.

The Agency sometimes sets New Chemical Exposure Limits (NCELs) for new chemicals regulated under TSCA. An NCEL is the concentration that a worker who makes or uses a chemical can be exposed to safely. To derive an NCEL for a potential carcinogen, the USEPA reportedly begins with the policy that a cancer risk of 10^{-4} is acceptable (USEPA 1995). But in some cases the Agency finds that the calculated NCEL may be difficult to attain or monitor. In such cases the risks to workers may be higher than 10^{-4} (Sellers 2015).

2.6 Superfund

The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), also known as Superfund, defines the significant risks at uncontrolled hazardous waste sites that must be cleaned up. The regulations at 40 CFR 300.430(e)(2)(i)(A) specify that remediation goals shall consider the following:

CERCLA/ SARA – 1980 / 1986	
Health based standards	✓
Balancing standards	
Technology based standards	

> *For known or suspected carcinogens, acceptable exposure levels are generally concentration levels that represent an excess upper bound lifetime cancer risk to an individual of between 10^{-4} and 10^{-6} using information on the relationship between dose and response. The 10^{-6} risk level shall be used as the point of departure for determining remediation goals ….*

[4] This discussion is adapted from: Sellers, K., 2015 (in press). *Product Stewardship, Life Cycle Analysis, and the Environment*. (Taylor & Francis/ CRC Press)

2.7 Inconsistent results

The different benchmarks for acceptable risks have led to some striking inconsistencies in the ways in which some chemicals are regulated in the United States Consider the example below, which contrasts risk management decisions under TSCA and the Safe Drinking Water Act (SDWA).

While the USEPA has not published a direct statement under TSCA on what level of risk is acceptable, it is interesting to compare risk-related benchmarks under TSCA to those under the SDWA[5].

When the exposure to a new chemical will be quite limited – or more specifically 'low release and exposure' (LoREX) – the manufacturer or importer can be exempt from TSCA regulations. Regulations at 40 CFR 723.50(2) specify the criteria for the LoREX exemption. They include the case where no exposure in drinking water would exceed a 1 milligram per year (mg/yr) estimated average dosage. While this exemption does not define serious human health effects or significant environmental effects to a degree that helps to explain the concept of "unacceptable risk" under TSCA, it does provide a point of reference: the risks from exposure to any compound at 1 mg/yr in drinking water are anticipated to be acceptable.

The USEPA has also considered the possible risk from chemicals in drinking water under the SDWA. A risk assessor working under USEPA guidelines has typically assumed that an adult drinks 2 liters of water per day (USEPA 2011). An adult drinking 2 liters of water per day for an entire year could drink water containing up to 0.0014 milligrams per liter (mg/L) of a chemical before reaching the LoREX criterion of 1 mg/yr of exposure:

2 liters water / day * 365 days/year * 1 year * 0.0014 milligrams / liter * = 1 mg/yr

The MCLs for 10 chemical (nonradionuclide) substances are below 0.0014 mg/L (USEPA 2013C). Put another way, for 13% of the chemicals regulated under the SDWA (that is, 10/76) the USEPA has found that exposure to 1 mg/yr in drinking water – which is considered to be a negligible exposure under the TSCA New Chemicals program – was not acceptable. If such chemicals were brought onto the market now, they could be exempted from regulation under TSCA.

[5] This discussion is adapted from: Sellers, K., 2015 (in press). *Product Stewardship, Life Cycle Analysis, and the Environment*. (Taylor & Francis/ CRC Press)

2.8 Summary

The level of risk considered to be acceptable varies widely between different federal regulatory programs. The risks we experience at work or by drinking from a public water supply can be on the order of $1x10^{-4}$ or even higher. Under other programs, such as the cleanup of hazardous waste sites, a risk level of $1x10^{-6}$ is the point of departure for determining the goals for cleanup though as long as excess lifetime cancer risk is equal to or less than $1x10^{-4}$ a site generally does not require cleanup. Perhaps most relevant to this discussion are the risk goals set under the Clean Water Act. Federal water quality criteria are typically based on a risk of $1x10^{-6}$; the USEPA has noted that criteria based on a 1/100,000 risk are acceptable for the general population as long as groups of people who may be more highly exposed (such as subsistence anglers) would encounter a risk less than or equal to $1x10^{-4}$.

3. Estimating risks: importance of underlying assumptions

The preceding paragraphs described the variation in one important assumption, the level of acceptable risk. That value may vary from 10^{-7} to more than 10^{-3}, depending upon the regulatory program and the context of the decision. Risk assessors must make other assumptions to estimate the possible risks from exposure to chemicals in the environment. These include assumptions about the degree of exposure. To illustrate the range of assumptions that can be factored into calculations of risks, Section 3.1 describes fish consumption estimates. Section 3.2 describes the effects of compounding a series of assumptions, if the assessor selects the most conservative value for each.

3.1 A closer look at one critical assumption: fish consumption

Calculations of the risk from eating fish containing chemicals in the environment typically reflect a simple assumption about the amount of fish eaten by each person per day or per year. But such values represent some complicated variables. Different people eat different amounts of fish. Those fish may come from different places, some very far from the area being considered in the risk assessment. The ways in which fish are cooked can decrease the amount of chemicals in the fish. The assumptions that are made to account for these variables and simplify the calculations can have a big effect on the calculated risk.

> 95th Percentile Values
> The 95th percentile value for a variable like fish consumption means that 95 out of 100 people eat less fish than that amount.

The amount of fish a person eats every day depends in part on geographic region, age, gender, and body size (USEPA 2011), as well as cultural or taste preferences. Estimates of fish consumption can also vary based on the way in which the fish consumption rate is estimated. A detailed discussion of all of those factors and their effect on fish consumption is beyond the scope of this white paper. But consider the values listed in **Table 6** (Washington State Department of Ecology 2013) for illustration.

Table 6 Variations in fish ingestion rates

Population	Key Variable	Fish	Mean fish ingestion (g/day)	95% Percentile (g/day)
Washington's Model Toxics Control Act (MTCA) Cleanup Regulation	Default fish consumption rate	All	54	
General population, Washington State, consumers only	NCI estimation method	All	19	57
Columbia River Tribes	All sources of fish	All	63	194
Tulalip Tribes	All sources of fish	All	82	268
Squaxin Island Tribe	All sources of fish	All	84	280
Suquamish Tribe	All sources of fish	All	214	797
Recreational Fishers, Washington State	Freshwater	All	6.0 to 22	42 to 67

How do we account for such varying rates of fish consumption in estimating risk and setting protective environmental standards? One way is to incorporate the range of values into risk calculations in a method known as probabilistic risk assessment. Another way is to pick a value for fish consumption that protects the majority of the population at the target excess lifetime cancer risk in order to set a criterion, and then to make sure that the standard represents a reasonable level of risk for more highly exposed groups of people. **Table 7** illustrates the results of a series of hypothetical calculations. It shows how the calculated risk varies with the amount of fish eaten, as described below.

Table 7 Excess Lifetime Cancer Risk versus Fish Consumption Rates

	MTCA Default	Washington State, mean	Washington State, 95th Percentile	Proposed regulation	Suquamish Tribe, 95th percentile
Fish consumption rate (grams per day)	54	19	57	175	797
Excess Lifetime Cancer Risk	1E-05	4E-06	1E-05	3E-05	1E-04
	3E-05	1E-05	3E-05	9E-05	4E-04
	9E-06	3E-06	1E-05	3E-05	1E-04
	3E-06	1E-06	3E-06	1E-05	5E-05
	7E-07	2E-07	7E-07	2E-06	1E-05

Five values are shown for fish consumption rate. These five values for the amount of fish that people in Washington might eat every day cover the range of values shown previously in Table 6. Included in Table 7 are the amounts eaten by fish consumers throughout Washington as represented by the MTCA default

value, fish consumers throughout Washington as represented by the mean rate of consumption and the 95th percentile, and the value of fish consumption included in the proposed criteria. The table also includes the amount eaten by members of the Suquamish tribe at the 95th percentile, who eat the largest amounts of fish of all the people in Washington State (Washington State Department of Ecology 2013).

The rows labelled excess lifetime cancer risk in Table 7 show how the calculated risk varies with the amount of fish eaten. In each row, the shaded box shows the group that was "assigned" a 1x10^{-5} (or 1E-05) risk. For example, calculations summarized in the first excess lifetime cancer risk row started with the assumption that the risk to people eating 54 grams per day of fish (Washington State MTCA default value) should be no more than 1x10^{-5} or 1E-05. The risk to the group that eats the most fish (Suquamish Tribe, 95th percentile) would then be no more than 1x10^{-4} or 1E-04 if all of the other variables in the calculation remained the same. Similarly, the last row in the table shows that if one were to base a standard on a 1x10^{-5} (or 1E-05) risk level to the most highly exposed people in the Suquamish Tribe (95th percentile) then the general population of fish eaters would be protected at the 7x10^{-7} level.

What do these calculations mean with respect to public policy? Water quality criteria based on the mean fish consumption rate in Washington and an excess lifetime cancer risk of 1E-05 present a risk that, even to the most highly exposed populations, is within the acceptable range as defined by USEPA (2000). The default fish consumption rate does not need to be raised to 175 grams per day to protect the people of Washington State from unreasonable risk.

3.2 Compounded conservatism

Conservative assumptions add up. If a decision maker chooses a conservative value for every variable in a risk calculation, the results will be far more protective than intended. Consider the hypothetical example of a risk assessment that is based on three independent and log-normally distributed parameters (Burmaster and Harris 1993). In the case of a fish consumption calculation, those parameters might be the amount of fish eaten each day, body weight, and the number of years over the course of a lifetime that people live in a certain place and eat fish from a local source. Each value represents the 95th percentile, or in other words that 9,500 out of 10,000 people have a lower exposure: they eat less fish, or do not eat fish from a stream for as many years, for example. Combining those three variables would result in a risk estimate that would fall at the 99.78th percentile of the resulting distribution. The risk to 9,978 out of 10,000 people would be lower than the allowable risk level used to establish the standard. Decisions made on the basis of this hypothetical calculation, which compounds conservative factors, would be far more protective than perhaps originally planned by the decision maker who intended to protect the average member of the population (or the 90th percentile or even the 95th percentile of the population) at the selected allowable risk level.

This may look like an academic calculation. Some readers may think that overestimating risks is a good thing because it allows us to be extra-cautious, and that regulatory decisions based on risk estimates should

be as conservative and protective as possible. But the consequences of such choices also need to be considered. There's a cost to reducing the levels of chemicals in the environment to meet more-stringent limits, a cost that may be measured in dollars, energy usage, or the risk of injury to workers who have the job of reducing the levels of those chemicals. Chemicals may be used to treat wastewater to meet lower standards, for example, and the sludge that results has to be trucked to a landfill or incinerated. Generating the power used to operate the wastewater treatment plant uses natural resources and creates air emissions. Each of these aspects of the life cycle of wastewater treatment operations, and their related risks, should be weighed against the value of regulatory decisions based on compounded conservatism.

Compounding the use of a high fish consumption rate, long duration of residence, upper percentile drinking water rate, and other high-end assumptions to estimate risks with a low target excess lifetime cancer risk will result in a water quality standard that is far more protective of the vast majority of the population than reflected by the target excess lifetime cancer risk. That additional degree of protection must be weighed against the risks and environmental impacts that would result from the additional treatment needed to meet such a standard.

4. Environmental Justice considerations

Environmental justice is, in the words of USEPA (2014),

> *… the fair treatment and meaningful involvement of all people regardless of race, color, national origin, or income with respect to the development, implementation, and enforcement of environmental laws, regulations, and policies. …. It will be achieved when everyone enjoys the same degree of protection from environmental and health hazards and equal access to the decision-making process to have a healthy environment in which to live, learn, and work.*

But how do we know what's fair treatment? The USEPA (2006) has developed guidelines relevant to risk-based decision-making. After defining the problem to be solved and collecting relevant information, we are to assess the potential for "adverse" environmental and human health effects or impacts, and to assess the potential for "disproportionately high and adverse" effects or impacts before deciding on a course of action.

Within the context of setting HHWQC within the State of Washington and the discussion in this white paper, the adverse human health effect of particular concern is cancer. At issue is whether the higher rates of fish consumption by Native Americans could lead to a disproportionate and unfair risk. The proposed criteria reflect two key assumptions: that citizens in Washington State consume 175 g/day of fish, and that $1x10^{-5}$ is the maximum acceptable level of risk. These two assumptions are each conservative and they need not be compounded in order to achieve environmental justice.

As demonstrated in Table 7, a standard based on the premise that those eating an average amount of fish each day would be protected to $1x10^{-5}$ risk level would assure that even the most highly exposed population, represented by the 95th percentile of the Suquamish Tribe, would encounter a risk of $1x10^{-4}$. Such a risk would not be "disproportionately high and adverse". As indicated in Section 2.2,

> *EPA also believes that criteria based on a 10^{-5} risk level are acceptable for the general population as long as States and authorized Tribes ensure that the risk to more highly exposed subgroups (sportfishers or subsistence fishers) does not exceed the 10^{-4} level.*

Further, the 10^{-4} risk level is embedded in many other standards, including drinking water; our standards for protecting workers on the job reflect the judgment that a 10^{-3} risk is acceptable. As a society, we accept that level of risk as reasonable.

Increasing the assumed amount of fish consumption or capping the acceptable level of risk is not necessary to develop standards that correspond to risks within acceptable bounds. Nor is it necessary to achieve environmental justice.

5. Putting environmental risks in perspective: every day risks

Consider how a $1x10^{-6}$ lifetime risk of developing cancer compares to risks we face in our daily lives. For ease of discussion, we can refer to mortality risks in terms of micromorts[6], units representing a one in one million chance of death. For example, one micromort is the risk incurred by the average person driving 240 miles in the United States. The micromort allows different kinds of risk to be compared on a similar scale. Motorcycling 20 miles or undergoing anesthesia are equivalent to 5 micromorts apiece, skydiving or running a marathon are equivalent to 7 micromorts apiece, and giving birth in the United States is equivalent to 210 micromorts (Blastland and Spiegelhalter 2014). When we compare a lifetime risk of developing cancer to such micromorts, we need to keep two important distinctions in mind. Not all cancers are fatal. And many of the micromort statistics described below represent the risk of death *each year*, not over the course of a lifetime.

In 2010, approximately 140,000 people died in the United States from unintentional injury-related deaths (e.g., poisoning, motor vehicle traffic, firearms, falls) (Murphy et al. 2013). This means that given a total population of 300 million people, the average American faced an unintentional injury-related mortality risk of approximately 467 micromorts per year in 2010, or 1.3 micromorts per day. In other words, about 413

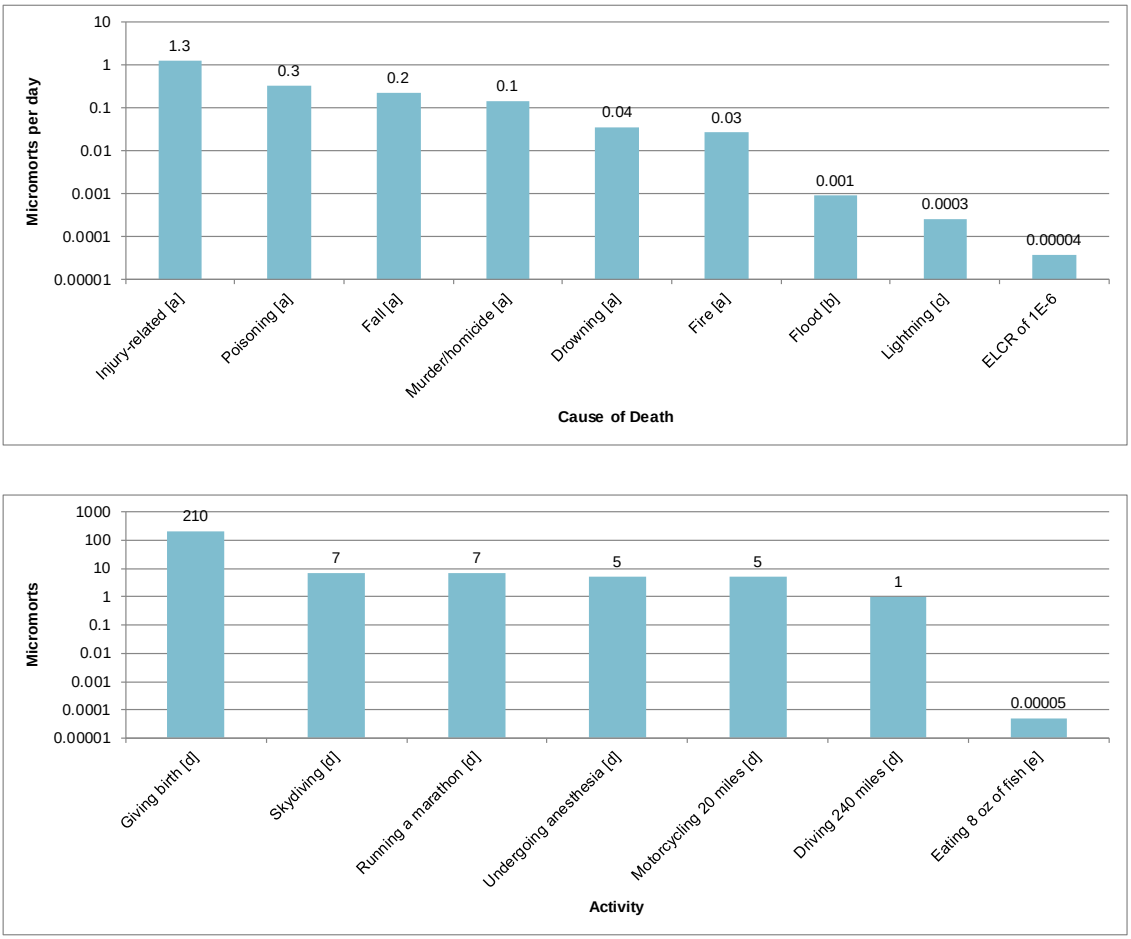
[6] A micromort is a unit of risk that represents a one-in-a-million ($1x10^{-6}$) probability of death. Risk assessors use micromorts to characterize and compare the riskiness of various day-to-day activities.

people die each day from an unintentional injury. This means that *every day*, *every American* has a risk of slightly greater than $1x10^{-6}$ of dying from unintentional injury.

Compare this to an excess lifetime cancer risk of $1x10^{-6}$, which (if we assume a lifetime corresponds to 70 years as does USEPA) translates to a worse-case 0.01 micromorts per year or 0.00004 micromorts per day; this is worse case from the perspective that not all cancers are fatal and the risks estimated by risk assessments are *upper bound estimates* of risk and *do not* represent *actual* risks. Thus, USEPA's definition of "acceptable" risk is several orders of magnitude below the average American's daily risk of dying from an unintentional injury; it is also approximately 3,500 times lower than the 2010 risk of dying from a murder/homicide (16,259 deaths or 0.1 micromorts per day), 20 times lower than the 2010 risk of dying from a flood (103 deaths or 0.001 micromorts per day) and 10 times lower than the 2010 risk of dying from a lightning strike (29 deaths or 0.0003 micromorts per day) in the United States (Murphy et al. 2013; NOAA 2014a,b) (**Figure 2**). This is consistent with the concept of $1x10^{-6}$ being a *de minimus* level of risk, because risks within this range are not risks that most members of the general public are concerned with and attempt to actively avoid.

Consider next that many regulatory agencies employ the USEPA-recommended $1x10^{-6}$ risk level to deriving HHWQC that relies on conservative upper-end values to estimate exposure. If one were to derive organism-only HHWQC by selecting a fish consumption rate of 175 g/day and targeting a risk level of $1x10^{-6}$, this means that a person would need to consume approximately 4,500 kilograms of locally-caught fish in his or her lifetime just to reach this *de minimus* level of risk, assuming ambient water always contains chemicals present at the resulting HHWQC. This also means that the risk associated with a single meal of fish would be $5x10^{-11}$, or 0.00005 micromorts, which for perspective should be noted is 20,000 times lower than the risk an average person faces when driving 250 miles in the United States (1 micromort) (**Figure 2**). Given that 175 g/day is an upper-end consumption rate estimate, the average member of the population would have an excess lifetime cancer risk lower than $1x10^{-6}$. For example, if we assume the average member of the population eats 8 g/day of fish, he or she would have an excess lifetime cancer risk of $5x10^{-8}$, roughly 20 times lower than the high-end consumer. If, on the other hand, one were to derive organism-only HHWQC by selecting an average fish consumption rate of 8 g/day and targeting a risk level of $1x10^{-6}$, the high-end consumer eating 175 g/day would have an excess lifetime cancer risk of $2x10^{-5}$, higher than $1x10^{-6}$ but still nearly an order of magnitude below the level USEPA (2000) recommends for highly exposed populations. Risk managers must make decisions such as these, recognizing that if highly exposed individuals are protected at $1x10^{-6}$, the average member of the population – and in fact the majority of the population itself – will have risks well below this *de minimus* level.

Figure 2 Common Risks Expressed as Micromorts



Notes:

[a] Murphy et al. (2013)

[b] NOAA (2015a)

[c] NOAA (2015b)

[d] Blastland and Spiegelhalter (2014)

[e] Assuming organism-only AWQC are based on a fish consumption rate of 175 grams per day and risk level of $1x10^{-6}$.

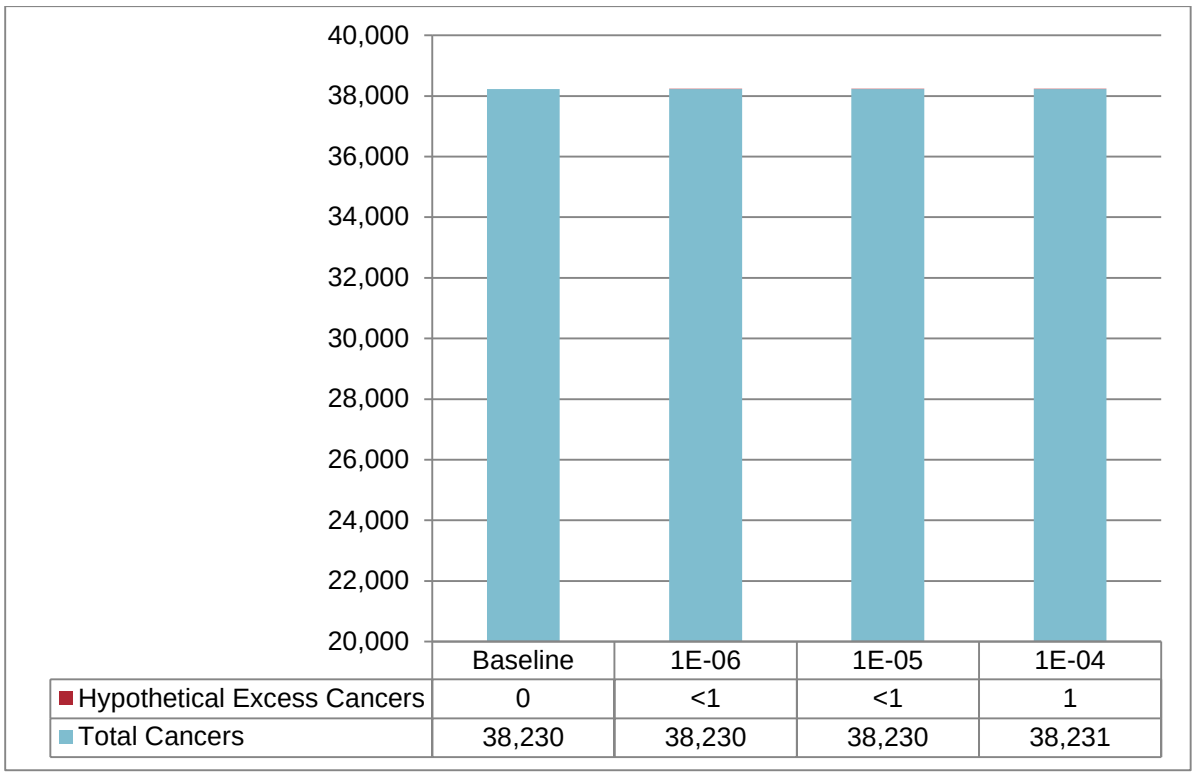
Another perspective when thinking about allowable risk is to consider the reduction or change in cancers associated with a particular allowable risk level. Allowable risk levels that result in large reductions in expected cancers clearly have a greater public health benefit than allowable risk levels that result in little

change. The average excess lifetime cancer risk can be combined with the estimated size of the population of Washington (7,061,530 in 2014) and the cancer rate in Washington in 2014 (38,230 new cancers) to see how large of a change in incidence is associated with using various allowable risk levels to set regulatory standards such as water quality criteria[7]. **Figure 3** shows that comparison.

The comparison illustrated in Figure 3 demonstrates that the annual increased incidence of cancer in the state of Washington associated with various alternative allowable cancer risks is very small when compared to the baseline incidence of cancer. This is true even at an allowable lifetime risk of $1x10^{-4}$ where 1 (and for the reasons described above, almost certainly less than 1) additional cancer may occur in the State compared to the 38,230 cased diagnosed in 2014. The change is two thousandths of a percent in overall incidence. Clearly, compared to total cancer incidence, the increases in cancers associated with the above allowable risk levels are small and are swamped by other causes of cancer. This finding is consistent with the comparisons of mortality risk associated with various allowable risk levels to mortality risk from various activities that are part of everyday life shown above.

[7] Assumptions used when deriving most criteria represent an upper percentile of the exposed population, not the average person in the population. To estimate the increased state-wide cancer incidence an average excess lifetime cancer risk needs to be used otherwise increased state-wide incidence will be overestimated. Based on the work we have completed using probabilistic approaches, criteria derived using the typical deterministic approach may overestimate the potential risk to an average member of the population by 10, 100, or more fold. Because a probabilistic evaluation of the proposed Washington criteria is beyond the scope of this paper an exact estimate of the excess lifetime cancer risk for an average Washingtonian could not be developed. However, we do know that the average Washingtonian eats about 19 grams of fish per day, not 175 as assumed by the proposed criteria. Therefore, that assumption ***by itself***, results in a nearly 10-fold overestimate of excess lifetime cancer risk for the average Washingtonian. Use of other conservative assumptions in the derivation of the proposed criteria means that the excess lifetime cancer risk for the average Washingtonian is more than 10-fold lower than the allowable excess lifetime cancer risk used to derive the proposed criteria. Based on the difference between the average fish consumption rate and the 175 grams per day assumed by proposed criteria, the increased incidence of cancers associated with different excess lifetime cancer risks was estimated by multiplying the expected annual cancer incidence associated with each of the excess lifetime cancer risks by the ratio of consumption rates (19 g/d/175 g/d = 0.109). The adjusted incidence of cancers based on a conservative estimate of excess lifetime cancer risk for the average Washingtonian are shown in Figure 3.

Figure 3 Comparison between Total Cancer Incidence and the Hypothetical Excess Annual Cancer Incidence Associated with Various Allowable Risk Levels



	Baseline	1E-06	1E-05	1E-04
Hypothetical Excess Cancers	0	<1	<1	1
Total Cancers	38,230	38,230	38,230	38,231

6. Health benefits of fish consumption

Finally, risk managers should also consider how the risks incurred from eating fish compare to the benefits gained. Researchers and public health officials have been aware for several decades that consumption of fish has associated with it many benefits. Early comparisons of those benefits to the potential risks associated with exposure to possible chemicals in the environment suggested that the benefits (specifically the reduced risk of mortality from coronary heart disease) far outweighed any increased cancer risks that might be associated with the allowable risk levels used in the derivation of HHWQC (e.g., $1x10^{-6}$, $1x10^{-5}$, and $1x10^{-4}$) (Anderson and Weiner 1995, Patterson 2002, Daviglus et al. 2002, Dourson et al. 2002, Anderson et al. 2002). A great deal of research continues on the health benefits and risks of consuming fish with measurable levels of chemicals. A literature search of publications since 2005 revealed over 400 citations, including three recent reviews by expert panels or recommendations by regulatory agencies (Nesheim and Yaktine 2007, WHO 2011, EFSA 2014). All of those recent expert reviews and regulatory agency recommendations continue to urge that people regularly consume fish. In fact, in the recommendation is that

the general population eat 1 to 2 meals per week and that pregnant women eat 2 to 4 meals per week because of the benefits to the infants they are carrying (EFSA 2014). Such benefits almost always outweigh the possible risks of chemical exposure.

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ATTACHMENT L

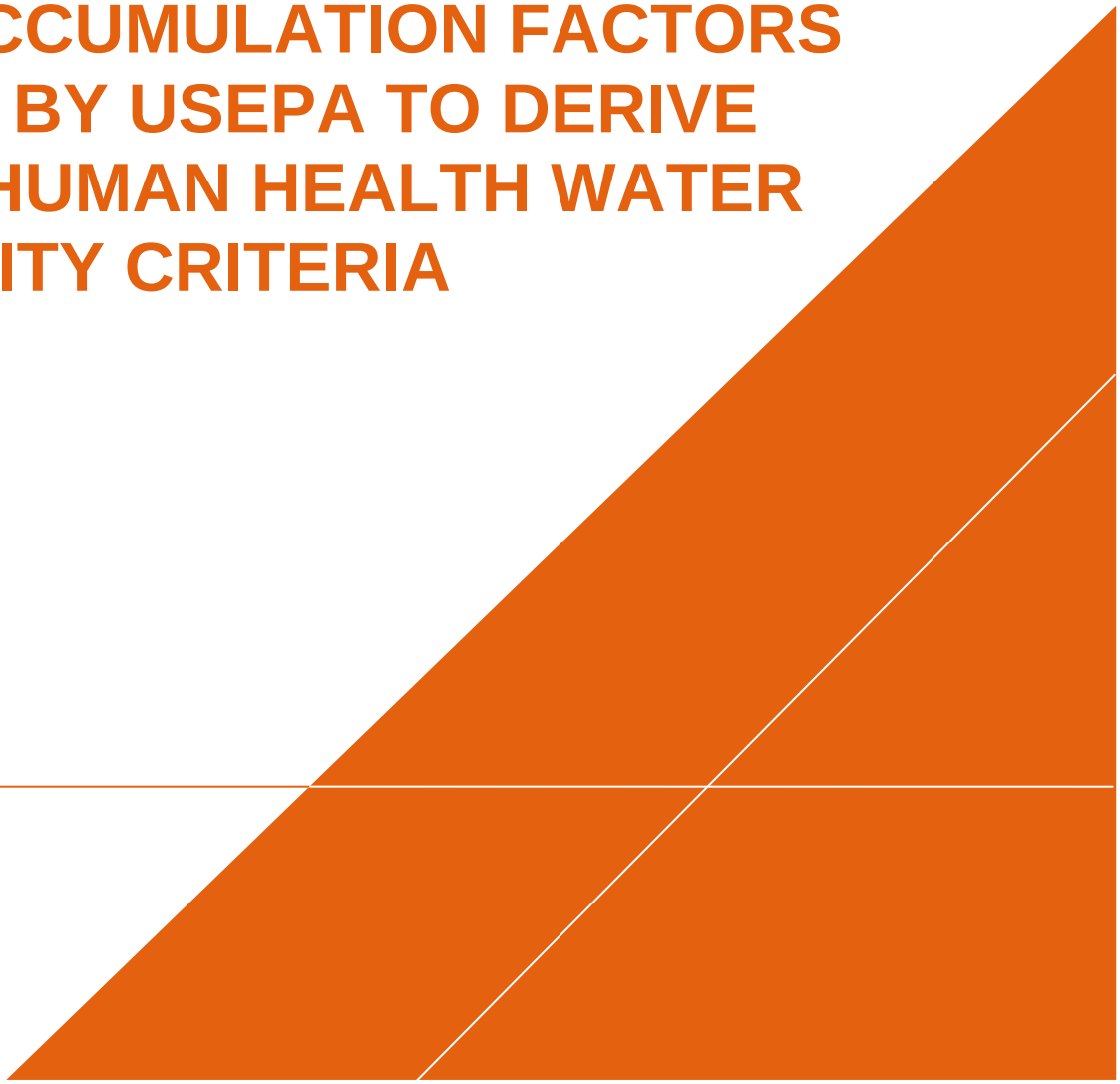
Refinement of Foodchain Multipliers and Bioaccumulation Factors Used by USEPA to Derive 2015 Water Quality Criteria

ARCADIS Design & Consultancy for natural and built assets

NCASI

REFINEMENT OF FOODCHAIN MULTIPLIERS AND BIOACCUMULATION FACTORS USED BY USEPA TO DERIVE 2015 HUMAN HEALTH WATER QUALITY CRITERIA

August 2018



REFINEMENT OF FOODCHAIN MULTIPLIERS AND BIOACCUMULATION FACTORS USED BY USEPA TO DERIVE 2015 WATER QUALITY CRITERIA

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CONTENTS

TABLES

FIGURES

APPENDICES

ACRONYMS AND ABBREVIATIONS

ATSDR	The Agency for Toxic Substances and Disease Registry
BAF	bioaccumulation factor
BaP	benzo(a)pyrene
BCF	bioconcentration factor
BSAF	biota-sediment accumulation factor
C_w^{fd}	concentration of chemical freely dissolved in the water column
DOC	dissolved organic carbon
FCM	foodchain multiplier
f_{fd}	fraction freely dissolved
f_l	fraction of tissue that is lipid
HHWQC	human health water quality criteria
HSDB	The United States National Library of Medicine's Hazardous Substances Data Bank
kd	dietary uptake constant
k_m	metabolic transformation constant
K_{ow}	n-octanol-water partition coefficient
NCASI	National Council for Air and Stream Improvement, Inc.
PCB	polychlorinated biphenyl
POC	particulate organic carbon
SOCW	sediment-water concentration quotient ($\prod_{socw}$)
TL	trophic level
USEPA	United States Environmental Protection Agency
$\prod_{socw}/K_{ow}$	sediment-water ratio

1 BACKGROUND

Estimating bioaccumulation of chemicals from ambient surface water into fish is a critical component in United States Environmental Protection Agency's (USEPA) derivation of national human health water quality criteria (HHWQC). USEPA's Technical Support Document, Volume 2 (USEPA 2003) defines bioaccumulation as "the uptake and retention of a chemical by an aquatic organism from all surrounding media (e.g., water, food, sediment)" and bioconcentration as "the uptake and retention of a chemical by an aquatic organism from water only" (USEPA 2003). USEPA's (2000) Human Health Methodology gives preference to bioaccumulation factors (BAFs) over bioconcentration factors (BCFs) because a BAF considers the potential chemical accumulation from all exposure pathways, not just water. However, relative to BCFs, which are typically derived in controlled laboratory studies, measured BAFs are rare and more difficult to estimate owing to the added complexity associated with the influence of food sources, sediment factors, and variable ambient conditions. Thus, USEPA's 2000 Human Health Methodology includes use of BCFs to estimate BAFs for criteria derivation. When USEPA updated its national HHWQC in 2015, a key change was using BAFs instead of BCFs to predict the uptake of a chemical by fish from surface water.

This report was developed to provide States and other stakeholders with additional background on the procedures USEPA followed to derive national BAFs used in the development of the 2015 national HHWQC (USEPA 2015a-e). The report begins with an overview of USEPA's BAF development methodology (Section 2). The report then presents in detail how USEPA developed national BAFs for four chemicals: benzo(a)pyrene, fluoranthene, di-n-butyl phthalate, and dieldrin (Section 3). Those four chemicals were selected to capture several of the different approaches used by USEPA to derive BAFs. The description of the BAF derivation process for each chemical is intended to be sufficiently detailed to allow interested readers to replicate USEPA's calculations for those four chemicals.

Many BAFs used by USEPA for derivation of the 2015 HHWQC were developed from data for polychlorinated biphenyls (PCBs) in the Great Lakes. As described in Section 4, incorporation in the BAF derivation procedure of assumptions that might be more representative of surface waters outside of the Great Lakes requires developing alternative inputs and running a bioaccumulation model. Recognizing that not all states will have the resources, expertise, or time, to become familiar with and run the model, alternative sets of foodchain multipliers (FCMs) are developed in Section 5 and presented in Appendix A. The different sets capture the FCMs for chemicals that have metabolic transformation rates that differ from PCBs and surface waters that have foodwebs and characteristics (e.g., temperature, sediment-water ratio) that differ from the Great Lakes. This information should allow states to select and apply FCMs to the derivation of BAFs that are more applicable and representative of surface waters in their states without having to run the bioaccumulation model.

2 USEPA BAF CALCULATIONS – OVERVIEW OF METHODOLOGY

USEPA estimated BAFs for updated 2015 HHWQC using USEPA's 2000 Methodology (USEPA 2000), its associated Technical Support Document, Volume 2: Development of National Bioaccumulation Factors (Technical Support Document, Volume 2) (USEPA 2003), and information distributed later as the 2016

Supplemental Information for USEPA's 2015 Human Health Criteria Update (USEPA 2016). USEPA followed the approach shown in Figure 1 (reproduced from Figure 3-1 of USEPA's Technical Support Document, Volume 2 [USEPA 2003]). USEPA used peer-reviewed, publicly available information to classify each chemical using this framework to derive BAFs, with some exceptions as noted in the following subsections. The framework provides guidance based on a chemical's properties and behavior in an aquatic environment. From the framework a procedure, and then one of up to four methods within a procedure, is selected for calculating a BAF for each trophic level within a foodweb. The four methods, in order of preference, are:

- Measured BAFs from a field study;
- BAFs derived from biota-sediment accumulation factors (BSAFs) from a field study;
- BAFs derived from BCFs from a laboratory study and, if necessary, multiplied by a foodchain multiplier (FCM); and
- BAFs calculated from a chemical's K_{ow} (n-Octanol/Water partitioning coefficient) and, if necessary, multiplied by a FCM.

USEPA's BAF derivation process normalizes measured BAFs and BCFs to predict accumulation assuming 100% of a chemical is dissolved in water and that fish are 100% lipid. USEPA refers to such normalized BAFs as "baseline BAFs". Because only a fraction of a chemical may be dissolved in ambient waters and because only a small fraction of the tissue of fish species in United States waters is comprised of lipid, USEPA then converts baseline BAFs to what it refers to as "national BAFs" by using national measured data on dissolved and particulate organic carbon in surface water to estimate the dissolved fraction of a chemical in United States surface waters and the lipid content of fish in each trophic level in United States surface waters.

Section 2.1 describes the BAF calculation methods used by USEPA and Section 2.2 provides a brief background for several of the key assumptions used to calculate BAFs.

2.1 BAF Calculation Methods

USEPA's stated preference is to use field-measured BAFs to estimate bioaccumulation of chemicals when deriving national HHWQC (USEPA 2003). However, field-measured BAFs are not available for most chemicals. In the absence of field-measured BAFs, USEPA relies on BCFs measured in laboratory studies or the K_{ow} of a chemical to predict a BCF and then uses a FCM to derive a BAF for a chemical from the BCF. USEPA (2000, 2003) identified log $K_{ow} \geq 4$ as the threshold for classifying a chemical as "moderately to highly hydrophobic" and for which exposure to chemicals through diet and other routes in addition to water can become important when estimating bioaccumulation. In other words, for chemicals with a log $K_{ow} < 4$, the BAF can be assumed to be equal to the BCF and FCMs are not used. For chemicals with log $K_{ow} \geq 4$, BAFs need to be developed and, depending upon USEPA method, FCMs may be needed. For each of the 94 chemicals for which USEPA updated HHWQC in 2015, Table 1 presents the log K_{ow}, the method USEPA used to derive the national BAF, the FCM for each trophic level and the BAF for each trophic level. Thirty-three chemicals had a log $K_{ow} \geq 4$ indicating that a FCM may be needed to derive a national BAF. For 12 of these 33 chemicals, USEPA used the field-measured BAF method. Four of the chemicals used the BCF method, eight used the BCF*FCM method, and nine used the K_{ow}*FCM method (Table 1). Of the four chemicals used as examples in this report, one had a field-

measured BAF (di-n-butyl phthalate), two had BCFs measured in a laboratory setting (BaP and fluoranthene), and the BCF for the fourth (dieldrin) was estimated based on K_{ow}.

The next three sections describe the methods used by USEPA to calculate baseline BAFs followed by a section that describes how baseline BAFs are converted national BAFs[1]. The national BAFs are used in the derivation of the 2015 national HHWQC.

2.1.1 Field BAF

The BAF Method uses measured BAFs derived from data obtained from field studies. A field-measured BAF is normalized by accounting for the portion of the chemical that is freely dissolved in the water in which the fish lives (referred to as fraction freely dissolved or f_{fd}) and the lipid content of the fish species (referred to as fraction lipid or f_ℓ). A normalized BAF is called a "baseline" BAF. The equation for calculating a baseline BAF using the BAF method is:

$$(\text{Baseline BAF})_i = \left[\frac{BAF_{Tt}}{f_{fd}} - 1\right] \times \frac{1}{f_\ell} \qquad \textit{eqn 1}$$

Where:

(Baseline BAF)$_i$ = baseline BAF for field sample i (L/kg-lipid);

BAF_{Tt} = total BAF from field sample (i.e. total concentration of chemical in tissue / total concentration of chemical in water [L/kg-tissue]);

f_{fd} = fraction of the total concentration of chemical in ambient water that is freely dissolved; and

f_ℓ = fraction of tissue in ambient fish that is lipid.

For some chemicals multiple baseline BAFs were available for a specific species or for several species within a trophic level. When more than one baseline BAF was available for a specific species, USEPA computed a species-specific baseline BAF using the geometric mean. If baseline BAFs were available for more than one species within a trophic level, then USEPA further averaged the BAFs across species within a trophic level to compute a trophic level-specific baseline BAF, again using the geometric mean. USEPA refers to the resulting BAF as the "trophic level-mean baseline BAF".

2.1.2 Lab BCF

The Lab BCF Method derives a national BAF from laboratory-measured BCFs and, depending upon chemical, with or without adjustment by a FCM. As with field-measured BAFs, a laboratory-measured BCF is normalized to account for the lipid fraction of the test species and the fraction of the chemical in water that is freely dissolved. For chemicals with log K_{ow} < 4, the baseline BAF is equal to the normalized BCF (i.e., the trophic level-specific FCMs are assumed to be equal to 1.0). For chemicals with log K_{ow} ≥ 4 but that are assumed by USEPA to have high metabolism, the baseline BAF is also equal to the normalized BCF. For chemicals with log K_{ow} ≥ 4 and that are assumed by USEPA to have low or unknown metabolism, the normalized BCF is multiplied by an FCM to derive the baseline BAF. The FCM varies

[1] The fourth method, the BSAF method, is not described because it was not used by USEPA to calculate national BAFs. The two compilations of data necessary to use the BSAF method – USEPA's Biota-Sediment Accumulation Factor Data Set, Version 1.0 (USEPA 2015a), and the U.S. Army Corps of Engineers' BSAF database (USACE 2015) – have not been peer-reviewed.

depending upon the K_{ow} of the chemical and trophic level. The equation for calculating a baseline BAF using the Lab BCF method is:

$$(\text{Baseline BAF})_{\text{i}} = (\text{FCM})_{\text{TL n}} \times \left[\frac{\text{BCF}_{\text{T}}\text{t}}{\text{f}_{\text{fd}}} - 1\right] \times \frac{1}{\text{f}_{\ell}} \qquad \textit{eqn 2}$$

Where:

(Baseline BAF)$_i$ = baseline BAF for laboratory sample i (L/kg-lipid);

FCM = foodchain multiplier for the trophic level associated with species from laboratory measurement;

$\text{BCF}_{\text{T}}\text{t}$= total BCF measured in the laboratory (i.e. total concentration of chemical in tissue ÷ total concentration of chemical in water [L/kg-tissue]);

f_{fd} = fraction of the total concentration of chemical in water that is freely dissolved; and

f_{ℓ} = fraction of tissue that is lipid.

Multiple Lab BCF method derived baseline BAFs are averaged using a geometric mean across species and then across trophic level to compute trophic level-mean baseline BAFs for each trophic level following the same procedure as described above for multiple field-measured BAFs.

2.1.3 K_{ow}

The K_{ow} Method derives a national BAF from a chemical's K_{ow} and, depending upon chemical, with or without adjustment by an FCM. For chemicals with log K_{ow} < 4, the baseline BAF is assumed to be equal to the K_{ow} (i.e., the trophic level-specific FCMs are assumed to be equal to 1.0). For chemicals with log K_{ow} ≥ 4 but that are assumed by USEPA to have high metabolism, the baseline BAF is also assumed to be equal to the K_{ow}. For chemicals with log K_{ow} ≥ 4 and that are assumed by USEPA to have low or unknown metabolism, the normalized BCF is multiplied by an FCM to derive the baseline BAF. The FCM varies depending upon the K_{ow} of the chemical and the trophic level. The equation for calculating a baseline BAF using the K_{ow} method is:

$$(\text{Baseline BAF})_{n} = (\text{FCM})_{\text{TL n}} \times \text{Kow} \qquad \textit{eqn 3}$$

Where:

(Baseline BAF)$_n$ = baseline BAF for trophic level n (L/kg-lipid);

(FCM)$_{TL\ n}$ = foodchain multiplier specific to trophic level n; and

K_{ow} = n-octanol-water partition coefficient (L/kg).

2.1.4 Converting Baseline to National BAFs

Sections 2.1.1 through 2.1.3 above describe the methods USEPA used to calculate trophic level-mean baseline BAFs. Trophic level-mean baseline BAFs are then converted to trophic level-specific national BAFs by accounting for national default values for lipid content of fish in each trophic level and a national default level for fraction of a chemical that is freely dissolved. Estimation of f_{fd} depends upon default concentrations of dissolved organic carbon (DOC) and particulate organic carbon (POC) in United States surface waters and the K_{ow} of each chemical (see equation 5, used to estimate f_{fd} below in Section 2.3.3). USEPA used the 50th percentile (median) DOC and POC concentrations as the national-level defaults. The equation for converting a trophic level-specific baseline BAF to a trophic level-specific national BAF is:

$$\text{National BAF}_{(\text{TL n})} = [(\text{Baseline BAF})_{\text{TL n}} \times (\text{f}_{\ell})_{\text{TL n}} + 1] \times (\text{f}_{\text{fd}}) \qquad \textit{eqn 4}$$

Where:

National $BAF_{(TL\ n)}$ = national trophic level-specific BAF (L/kg-tissue);
$(Baseline\ BAF)_{TL\ n}$ = mean baseline BAF for trophic level "n" (L/kg-lipid);
$f_{\ell(TL\ n)}$ = fraction of tissue that is lipid in aquatic organisms in trophic level "n"; and
f_{fd} = fraction of the total concentration of chemical in ambient surface water that is freely dissolved.

When national trophic level-mean BAFs are not available for all three trophic levels, USEPA applies the available national trophic level-mean BAFs to all trophic levels. If a single national trophic level-mean BAF is available, that is used to predict bioaccumulation in all trophic levels. If two national trophic level-mean BAFs are available, the geometric of those two national trophic level-mean BAFs is used to predict bioaccumulation in all trophic levels.

2.2 Key Assumptions Used to Derive BAFs

2.2.1 K_{ow}

Bioaccumulation of non-ionic hydrophobic chemicals is assumed to be closely related to a parameter known as the n-octanol-water partition coefficient, or K_{ow}. The K_{ow} is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase octanol/water system. An increase in K_{ow} represents an increase in lipophilicity and the increased potential for bioaccumulation. In the absence of measured BAFs and BCFs a chemical's K_{ow} can be used to estimate BAFs and BCFs. USEPA selected K_{ow}s from the Agency for Toxic Substances and Disease Registry (ATSDR) or The United States National Library of Medicine's Hazardous Substances Data Bank (HSDB) with preference given to ATSDR. An average K_{ow} was computed if a range or multiple K_{ow}s were reported from the selected source.

2.2.2 Foodchain Multiplier

The FCM is selected from Table 4-6 in USEPA's Technical Support document (USEPA 2003), also provided in Table 1 in USEPA (2016) and in this report (Table 2), using the chemical's log K_{ow} and linear interpolation (USEPA 2003, p. 4-39; USEPA 2016, p. 8). Chemicals with a log $K_{ow} < 4$ are assumed by USEPA to have an FCM equal to 1.0. Additional detail regarding the derivation of FCMs is provided in Section 4 of this report.

2.2.3 Fraction Freely Dissolved

The fraction of the concentration of chemical in water that is freely dissolved (f_{fd}) is included in both the BCF method and the national BAF equations. Distinguishing the freely dissolved fraction from the total concentration in the water column (which can include chemical bound to particulate that is not, or is less, bioavailable) is important when estimating BCFs and BAFs. To estimate f_{fd} in ambient United States surface water, USEPA uses national default DOC and POC concentrations. The assumed national default concentration of DOC is 2.9×10^{-6} kg/L [= 2.9 mg/L] and of POC is 0.5×10^{-6} kg/L [= 0.5 mg/L] (USEPA 2003, 2016). The equation used to compute f_{fd} is:

$$f_{fd} = \frac{1}{1+POC \times K_{ow} + DOC \times 0.08 \times K_{ow}} \qquad \textit{eqn 5}$$

Where:

f_{fd} = fraction freely dissolved;
POC = concentration of particulate organic carbon in water (kg of POC per liter of water) (kg/L);
DOC = concentration of dissolved organic carbon in water (kg of DOC per liter of water) (kg/L); and
K_{ow} = n-octanol-water partition coefficient.

USEPA's HHWQC procedure includes the ability of States to use alternate, State-specific DOC and POC concentrations to derive State-specific HHWQC. The focus of this report is on refinement of FCMs used to derive HHWQC; this report does not review the process used by USEPA to develop alternate HHWQC based on DOC and POC concentrations that differ from the national default DOC and POC concentrations. An example of such State-specific refinement can be found in FDEP (2016).

2.2.4 Lipid Content

Lipid content is the fraction of fish tissue that is assumed to be comprised of lipid. Because USEPA's goal was to establish trophic level-specific BAFs for each trophic level, assuming available data allow, USEPA needed to develop estimates of the lipid content of fish in each trophic level. USEPA followed the hierarchical steps listed below to determine the default national trophic level-specific lipid content.

1. Use measured values if provided.
2. Select a lipid content based on species from Tables 4-5 and 6-3 in the TSD (USEPA 2003, p. 4-37, 6-18).
3. Use an average species value from all studies in database with reported values.
4. Apply national lipid fractions based on assigned tropic level (f_ℓ(TL2) = 0.019, f_ℓ(TL3) = 0.026, f_ℓ(TL4) = 0.030).

USEPA's HHWQC procedure includes the ability of States to use alternate, trophic level-specific lipid fractions to derive State-specific HHWQC. The focus of this report is on refinement of FCMs used to derive HHWQC; this report does not review the process used by USEPA to develop alternate HHWQC based on alternate trophic level-specific lipid fractions. An example of such State-specific refinement can be found in FDEP (2016).

2.2.5 Trophic Level

Trophic level assignment information was primarily obtained from the USEPA (2014) NHANES Fish Consumption Rate Report and Fishbase.org and used to determine trophic levels of organisms in the BCF and BAF data sources (USEPA 2014; Froese and Pauly 2015). When no primary source was available, an expert fishery biologist and an expert invertebrate zoologist provided trophic level identifications. These experts checked all trophic level identifications for correctness and consistency.

3 NATIONAL BAF CALCULATIONS FOR FOUR CHEMICALS

The steps USEPA used to calculate national BAFs for benzo(a)pyrene, fluoranthene, di-n-butyl phthalate, and dieldrin are described in this section.

USEPA searched peer-reviewed journal articles, federal and state reports, and databases to obtain input parameters for each chemical. USEPA was not able to locate peer-reviewed, field-measured BAFs, BSAFs, or lab-measured BCFs for all three trophic levels (TL2, TL3, and TL4) for any of the four chemicals discussed in the subsequent sections. The BAF calculation method for each chemical was selected using the procedures and methods outlined in Figure 1 based on each individual chemical's physical properties and based on that chemical's behavior (i.e., it's ionic and hydrophobic tendencies, K_{ow}, and ability to be metabolized). Specific calculations of each BAF are outlined in Sections 3.1 to 3.5.

3.1 Benzo(a)pyrene

Benzo(a)pyrene (BaP) is a nonionic organic chemical (USDHHS 2010a) and was classified by USEPA as having moderate-high hydrophobicity with a log K_{ow} of 6.06 (ATSDR 1995) and to have high metabolism (USEPA 2015). USEPA was unable locate peer-reviewed field-measured BAFs for BaP but was able to locate peer-reviewed lab BCF data. Given those physical characteristics and the availability of laboratory measured BCFs, according to USEPA's BAF method selection framework, USEPA should have used the Lab BCF method in Procedure #2 to develop national BAFs for BaP (Figure 1). However, for reasons that remain unclear, USEPA instead used the Lab BCF*FCM method within Procedure #1 (Figure 1) to derive a national BAF of 3900 (L/kg) for all three trophic levels. Because USEPA was only able to locate laboratory BCFs for TL2 and TL3, but not TL4, USEPA used the geometric mean of the national TL2 and TL3 BAFs as the national BAF for all three trophic levels. The specific steps used by USEPA to derive the national BAF for BaP are briefly described below and presented in Tables 3a and 3b:

1. Twenty-seven laboratory measured BCFs were identified from five peer-reviewed papers (Landrum and Poore 1988; McCarthy 1983; Gossiaux et al 1996; Jimenez et al 1987[2]; Spacie et al 1983). Twenty-three BCFs were from TL2 organisms including amphipod (*Pontoporeia hoyi*), mayfly (*Hexagenia limbate*), shrimp (*Mysis relicta*), water flea (*Daphnia magna*), and zebra mussel (*Dreissena polymorpha*) (Table 3a). Four BCFs were from bluegill sunfish (*Lepomis macrochirus*), a TL3 organism.
2. Each of the 27 laboratory measured BCFs was converted to a baseline BAF using equation 2 shown above. (Table 3a). The process includes normalizing each laboratory measured BCF such that it is expressed on a freely dissolved and 100% lipid basis. If the laboratory study reported the freely dissolved concentration or the lipid content of the species tested in the laboratory, or both, those values were used to express the laboratory BCF on a freely dissolved and 100% lipid basis. If freely dissolved concentrations were not reported and concentrations of DOC and POC in the laboratory test water were not reported, USEPA estimated a freely dissolved concentration by assuming the concentration of DOC and POC in laboratory water was equal to the median concentrations reported in ambient waters of the United States (DOC= 2.9 mg/L and POC = 0.5 mg/L] using equation 5 shown above[3]. If lipid content was not reported, USEPA used the step-wise process described in Section

[2] Jimenez et al. (1987) report a BCF of 608 L/kg but the database used by USEPA lists a BCF of 842 L/kg for that study. The calculations presented in this section are based on the BCF of 608 L/kg used by USEPA and not the BCF 842 L/kg reported in Jimenez et al. (1987).

[3] As discussed in more detail near the end of Section 5, USEPA's assumption that laboratory water had a median DOC and POC concentration equal to ambient water likely overestimates BCFs if filtered was used in the laboratory study, which in turn, could result in lower than necessary HHWQC. Accounting for this potential bias would require making a more accurate estimate of the DOC and POC in laboratory waters and adjusting the BCF accordingly.

2.2.4 above to select a lipid fraction. The FCMs used by USEPA in the baseline BAF equation are described in more detail in Section 2.2.2 above. The resulting normalized BCFs for each of the 27 laboratory measured BCFs are shown in Table 3a.

3. Geometric mean baseline BAFs were then calculated first by species resulting in six species-specific baseline BAFs (five in TL2 and one in TL3, Table 3a) and then by trophic level (Table 3a), resulting in a trophic level-specific baseline BAF of 862,368 L/kg-lipid for TL2 and a trophic level-specific baseline BAF 120,798 L/kg-lipid for TL3.
4. National BAFs for TL2 and TL3 were then calculated from the baseline BAFs using equation 4 using a default national fraction freely dissolved of 0.5433 and national default fraction lipid of 0.019 and 0.026 for TL2 and TL3, respectively (Table 3b).
5. The final national BAF for benzo(a)pyrene of 3,900 L/kg was calculated as the geometric mean of the TL2 (8,900 L/kg) and TL3 (1,700 L/kg) national BAFs (Table 3b).

3.2 Fluoranthene

Fluoranthene is a non-ionic chemical (USDHHS 2010b) and was classified by USEPA as having moderate-high hydrophobicity with log K_{ow} = 4.9 (ATSDR 1995) with high metabolism (NOAA n.d.). USEPA was not able to locate peer-reviewed, field-measured BAFs, BSAFs, or lab-measured BCFs for all three trophic levels (TL2, TL3, and TL4) but was able to locate lab-measured BCFs for trophic level 2 organisms. Therefore, USEPA used the BCF method within Procedure #2 (Figure 1) with the TL2 BCFs available for fluoranthene to derive a national BAF of 1,500 (L/kg) for all three trophic levels. The specific steps USEPA used to derive the national BAF for fluoranthene are briefly described below and in Tables 4a and 4b.

1. Three BCFs were derived from one literature study (Sheedy et al 1998) on an oligochaete (*Lumbriculus variegatus*) a TL2 organism[4].
2. Each of the normalized laboratory BCFs was converted to a baseline BAF using equation 2 shown above. (Table 4a). The process includes normalizing each laboratory measured BCF such that it is expressed on a freely dissolved and 100% lipid basis. If the laboratory study reported the freely dissolved concentration or the lipid content of the species tested in the laboratory, or both, those values were used to express the laboratory BCF on a freely dissolved and 100% lipid basis. If freely dissolved concentrations were not reported and concentrations of DOC and POC in the laboratory test water were not reported, USEPA estimated a freely dissolved concentration using the same process described above for BaP. If lipid content was not reported, USEPA used the step-wise process described in Section 2.2.4 above to select a lipid fraction. The FCMs used by USEPA in the baseline BAF equation are described in more detail in Section 2.2.2 above. The resulting normalized BCFs for each of the three measured BCFs are shown in Table 4a.
3. A geometric mean baseline BAF was then calculated (Table 4a) resulting in a baseline BAF of 80,714 L/kg-lipid (Table 4a).

[4] Sheedy et al (1998) exposed the study organism to fluoranthene for a relatively short duration (96 hours) suggesting that the resulting BCFs may be biased low.

4. A national BAF for TL2 of 1,500 L/kg was then calculated from the baseline BAF using equation 4 with a default national fraction freely dissolved of 0.9451 and national default fraction lipid of 0.019 (Table 4b).
5. The final national BAF for fluoranthene for trophic levels was set equal to 1,500 L/kg, the national BAF based on TL2 organisms (Table 4b).

3.3 Di-n-Butyl Phthalate

Di-n-Butyl is a non-ionic organic chemical (USDHHS 2010c) and was classified by USEPA as having moderate-high hydrophobicity with log K_{ow} = 4.21 (ATSDR 2001) with high metabolism (Gobas et al. 2003; Mankidya et al. 2013). USEPA was not able to locate peer-reviewed, field-measured BAFs or lab-measured BCFs for all three trophic levels (TL2, TL3, and TL4) but USEPA was able to locate field-measured BAFs for trophic levels 3 and 4. Therefore, USEPA used the BAF method to estimate for the reported trophic levels by calculating the geometric mean of the TL3 and TL4 BAFs for di-n-butyl phthalate (Arnot and Gobas 2006; Environment Canada 2006) to derive the national BAF of 2,900 L/kg for this chemical. The specific steps in this procedure are described below and in Table 5a and 5b.

1. Eight BAFs were derived from two literature studies (Gobas et al 2003; Mackintosh 2002). Two BAFs were from TL3 organisms including whitespotted greenling (*Hexogrammos stelleri*) and English Sole (*Pleuronectes ventulus*) (Table 5a). Six BAFs were from TL4 organisms including Pacific staghorn sculpin (*Leptocottus armatus*), pile perch (*Rhacochilus vaccu*), spiny dogfish (*Squalus acanthias*), and striped seaperch (*Embiotoea lateralis*).
2. Each of the eight laboratory measured BAFs was converted to a baseline BAF using equation 1 shown above. (Table 5a). The process includes normalizing each measured BAF such that it is expressed on a freely dissolved and 100% lipid basis. If the study reported the freely dissolved concentration or the lipid content of the species, or both, those values were used to express the BAF on a freely dissolved and 100% lipid basis. If freely dissolved concentrations were not reported and concentrations of DOC and POC in ambient water were not reported, USEPA estimated a freely dissolved concentration using the same process described above for BaP. If lipid content was not reported, USEPA used the step-wise process described in Section 2.2.4 above to select a lipid fraction. The resulting normalized BAFs for each of the eight measured BAFs are shown in Table 5a.
3. The baseline BAF for each data point was calculated using equation 1 (Table 5a).
4. Geometric mean baseline BAFs were then calculated first by species (Table 5a) and then by trophic level (Table 5a), resulting in a trophic level-specific baseline BAF of 142,876 L/kg-lipid for TL3 and of 74,484 L/kg-lipid for TL4.
5. National BAFs for TL3 and TL4 were then calculated from the baseline BAFs using equation 4 (Table 5b) with a default national fraction freely dissolved of 0.988 and national default fraction lipid of 0.026 for TL3 and 0.03 for TL4.
6. The final national BAF for di-n-butyl phthalate of 2,900 L/kg was calculated as the geometric mean of the TL3 (3,700 L/kg) and TL4 (2,200 L/kg) national BAFs (Table 5b).

3.4 Dieldrin

Dieldrin is a nonionic organic chemical (USDHHS 2014) and was classified by USEPA as having moderate-high hydrophobicity with a log K_{ow} of 6.2 (ATSDR 2002) and to have low or unknown metabolism. Given those characteristics, and because USEPA was unable to find any field-measured BAFs or laboratory-measured BCFs, USEPA used the K_{ow}*FCM method within Procedure #1 (Figure 1) to derive national BAFs for dieldrin of 14,000 (L/kg) for TL2, 210,000 (L/kg) for TL3, and 410,000 (L/kg) for TL4 (Table 6). The specific steps USEPA used to derive the national BAF for dieldrin are briefly described below and in Table 6.

1. The baseline BAF for each trophic level was calculated using equation 3, assuming a log K_{ow} of 6.2 and FCMs of 1, 11.2, and 18.5 for TL2, TL3, and TL4, respectively (Table 6). The derivation of FCMs used by USEPA are described in Section 2.2.2 above.
2. National BAFs of 14,000 (L/kg), 210,000 (L/kg), and 410,000 (L/kg) for TL2, TL3, and TL4, respectively, were calculated using equation 4 (Table 6). The freely dissolved concentration of dieldrin in ambient surface water was estimated using equation 5 and assuming a log K_{ow} of 6.2 and national default median concentrations of DOC (2.9 mg/L) and POC (0.5 mg/L). The lipid content of fish was assumed to be equal to the national default lipid fractions of 0.019, 0.026 and 0.030 for TL2, TL3 and TL4, respectively (Table 6).

4 REFINING FOODCHAIN MULTIPLIERS AND BIOACCUMULATON FACTORS

This section describes the process and some of the key assumptions used by USEPA to develop FCMs. This section also discusses why some of those assumptions are not representative of the characteristics of many of the chemicals to which USEPA applied FCMs nor to many waters of the United States. The section concludes by showing how assumptions more representative of the characteristics of the three example chemicals[5] for which USEPA used FCMs to derive national trophic level-specific BAFs affect the FCM and the resulting national trophic level-specific BAF and resulting HHWQC.

USEPA used a foodweb model (Gobas 1993) parameterized for PCBs in a Great Lakes foodweb and fish tissue data to calculate FCMs for TL2, TL3, and TL4 (USEPA 2003). USEPA (2003) defines foodchain multipliers as “a measure of the chemical’s tendency to biomagnify in aquatic foodwebs” and provides the following equation:

$$FCM = \frac{Baseline\ BAF}{K_{ow}} \approx \frac{Baseline\ BAF}{Baseline\ BCF}$$

USEPA considered the models of both Gobas (1993) and Thomann et al. (1992) for development of FCMs, ultimately deciding to use the Gobas (1993) model for reasons described in USEPA (2003). Many

[5] Section 3 describes USEPA’s derivation of national BAFs for four chemicals (benzo(a)pyrene, fluoranthene, di-n-butyl phthalate, and dieldrin). This section, and the remainder of the report, develops alternative FCMs, BAFs and HHWQC for only three of the four example chemicals (benzo(a)pyrene, fluoranthene, and dieldrin) because those are the only three example chemicals for which USEPA used FCMs to develop national BAFs. Field-measured BAFs were available for di-n-butyl phthalate precluding the need to use FCMs to develop a national BAF for di-n-butyl phthalate.

of the values and assumptions used to parameterize the model for PCBs in the Great Lakes are likely different from the values and assumptions that would be used to represent other chemicals in surface waters and foodwebs in other locations in the United States.

The key input parameters are described below and summarized in Table 7. Arcadis input the values and assumptions for these key parameters as described in Gobas (1993) into the spreadsheet model, which is available online, in an effort to reproduce the FCMs published by USEPA (USEPA 2016).

4.1 Sediment-Water Ratio

USEPA describes the sediment-water concentration quotient ($\prod_{socw}$) as "the ratio of the chemical concentrations in the sediments (expressed on an organic carbon basis) to those in the water column (expressed on a freely dissolved basis)". USEPA reviewed data sets from Lake Ontario, Hudson River, and Green Bay in the Lake Michigan ecosystem to determine $\prod_{socw}$. USEPA's review concluded that $\prod_{socw}$ is strongly dependent on the K_{ow} and calculated an average value of 23 for the $\prod_{socw}/K_{ow}$ ratio (referred to in this report as the "sediment-water ratio").

USEPA acknowledges there is very large variability in $\prod_{socw}$ across ecosystems. USEPA also presents simulations showing that constant loading of a chemical with a log K_{ow} of 6 results in a maximum $\prod_{socw}/K_{ow}$ ratio of 4.9 (see Figure 4-5 of USEPA 2003). USEPA also states that with continued loading, sediment concentration will increase until a steady state condition is reached with a $\prod_{socw}/K_{ow}$ ratio in the 2 to 10 range. It would seem that the estimated $\prod_{socw}/K_{ow}$ ratio of 23 is only applicable to chemicals that have high historic loading followed by a large reduction in loading (e.g., PCBs in the Hudson River). Therefore, it is likely not applicable to other waterbodies in other areas of the United Sates. The $\prod_{socw}/K_{ow}$ ratio has a substantial effect on the FCMs of the three example chemicals in this report (Table 8) because the increase in benthic tissue concentrations from sediment cause an increase in tissue concentrations that cascade up the foodweb.

USEPA used three datasets to determine a default sediment-water ratio. These data sets were from areas of high historical loadings: Lake Ontario (Oliver and Niimi 1988), Hudson River (USEPA 1997, USEPA 1998), and Green Bay in the Lake Michigan ecosystem (www.epa.gov/grtlakes/gbdata/). The Green Bay and Hudson River data sets contained data for PCBs only, and the Lake Ontario data set contained data for chlorinated pesticides and PCBs (USEPA 2003, Table 4-4). For these three waters, USEPA identified a range of average sediment-water ratios: from 4.49 to 10.3 for Green Bay, and 14.3 to 48.4 for the Hudson River. The sediment-water ratio for Lake Ontario was 23.4. USEPA selected 23 as the default sediment-water ratio, which is the overall average of the sediment-water ratios from the above datasets. However, the default of 23 is likely high for most waters of the United States given that it is based on waters that are known to have had substantial historical loadings of contaminants and the sediment-water ratio is likely not at equilibrium.

Based on the information summarized above, this report uses sediment-water ratios of 23, 10, and 2 (Table 7) to represent the range of ratios that may be present in waters of the United States.

4.2 Chemical Concentrations in Sediment and Water Column

In deriving the FCMs, 1 ng/L (concentration of chemical freely dissolved in the water column, C_w^{fd}) is used. USEPA (2003) states that the corresponding chemical concentration in the sediment is calculated by using the $\prod_{socw}/K_{ow}$ ratio = 23 relationship, or C_s (ng/kg) = 23 (L/kg oc) * K_{ow} * (1 ng/L) * f_{oc} (kg oc/kg) * 0.001 (kg/g).

4.3 Organic Content of Water

The Gobas (1993) model takes the total concentration of the chemical in the water that is input to the model and, before doing any predictions, performs a bioavailability correction by calculating the C_w^{fd}. The C_w^{fd} is then used in all subsequent calculations by the model. The bioavailability correction relies on the DOC concentration in the water column. The smaller the DOC concentration, the greater the fraction of the chemical that is freely dissolved in the water column, and more of the chemical is considered to be bioavailable. When developing FCMs, USEPA needed to run the Gobas model assuming all of a chemical was dissolved in the water column. USEPA (2003) set the concentration of the DOC in the model to an extremely small number, $1.0x10^{-30}$ kilograms per liter (Table 7). By setting the concentration of the DOC to $1.0x10^{-30}$ kilograms per liter, the total concentration of the chemical input into the model becomes essentially equal to the C_w^{fd}.

4.4 Rate of Metabolism in Forage and Piscivorous Fish

The FCMs developed by USEPA (2003, 2016) assume no metabolic transformation of a compound by fish and shellfish[6]. That is, the metabolic transformation constant (k_m) is set to zero in the model when FCMs are calculated in part because information on metabolic transformation was lacking for many compounds when the model was parameterized (i.e., in the early 1990's) and also because the model was parameterized for PCBs, which are assumed to have relatively low metabolic transformation. Thus, the assumption of zero for the metabolic transformation rate constant is not unreasonable for PCBs (Gobas 1993). However, USEPA applies the FCMs developed using the assumption of zero for the metabolic transformation constant to derive HHWQC for many compounds that differ from PCBs and are likely to be metabolized by fish or shellfish or both. Additionally, a great deal more information on metabolic transformation rate constants is now available than was in the early 1990's. Arnot et al. (2008) produced a database of metabolic transformation rate constants for organic chemicals. Therefore, the assumption of zero metabolism is not only incorrect for many compounds, but data are available to estimate metabolic transformation of many compounds including for halogenated organics, phenyls, dioxins, furans, hydrocarbons, amines, imides, alcohols, phenols, ethers, ketones, and esters.

To evaluate the effect of incorporating metabolism into the Gobas (1993) model used to calculate FCMs, k_ms were obtained for benzo(a)pyrene, fluoranthene, and dieldrin. These chemical-specific k_ms were

[6] Because the FCMs assume no metabolism, USEPA's BAF derivation procedure (Figure 1) includes a decision point based on metabolism. That decision point precludes the use of FCMs when developing BAFs for chemicals that have high metabolism. In other words, for such chemicals, the BAF can be assumed to be equal to the BCF.

obtained from the database in Arnot and Gobas (2008) and normalized to the specific water temperature used in the model and the weights of each species in the foodweb. Table 9 summarizes K_ms available in Arnot and Gobas (2008) for the three example compounds. Table 10 presents the organism weight and temperature normalized K_ms for the three example compounds in all three foodwebs.

Many (if not most) chemicals undergo transformation. When transformation is accounted for and is substantial, it appears that FCMs can be less than 1.0, as demonstrated for the above three compounds (Table 8) and even for those chemicals that were not identified as "highly metabolized" by USEPA.

4.5 Additional Environmental Parameters and Conditions

USEPA (2003) used the following environmental parameters and conditions to determine FCMs (Table 7):

- Mean water temperature: 8°C;
- Organic carbon content of the sediment: 2.7%;
- Density of lipids: 0.9 kg/L; and
- Density of organic carbon: 0.9 kg/L.

The water temperature used by USEPA (8°C) is cooler than waters in other areas of the United States, particularly in the south. Water temperature is used in an equation that calculates the dietary uptake constant (kd) in the model. Using USEPA's set of default assumptions, the effect of increasing water temperature is to increase the FCMs because the increased temperature increases the dietary uptake (Table 8). Metabolic transformation rate also increases with increasing temperature, but because USEPA's default assumptions assume no metabolic transformation, FCMs can only increase with increasing temperature (compare FCMs in Appendix A tables at 8° and 16°C that assume no metabolism [k_m=0]). When metabolic transformation is included in the bioaccumulation model, FCMs can decrease with increasing temperature. The amount of decrease depends upon the magnitude of metabolic transformation. Because temperature varies across surface water in the United States, the effect of two different temperatures (8°C and 16°C) on FCMs are evaluated for the three example chemicals. Sediment organic carbon concentration does not affect FCMs. Density of lipids and density of organic carbon are not water body specific assumptions and are not expected to vary among surface waters. The latter three model parameters were not changed as part of the FCM refinement presented in this report.

4.6 Foodweb Structure

USEPA (2003) uses the mixed foodweb structure from the Lake Ontario ecosystem (Flint 1986; Gobas 1993) as the representative foodweb for determining FCMs for the national methodology. USEPA notes that there are large differences in foodwebs across the country and, for this reason, strongly encourages States and Tribes to make site-specific modifications to USEPA's national BAFs (USEPA 2000).

Consistent with that USEPA encouragement, this report evaluates FCMs using the Lake Ontario foodweb and two alternative foodwebs: a pelagic and a benthic based warm freshwater foodweb (Tables 11a and 11b). A warmwater foodweb comprised of warmwater species (e.g., sunfish, largemouth bass, catfish) was developed to better represent ambient waters in other parts of the United States. The base of one version of the warmwater foodweb is primarily benthic species (e.g., crayfish). This foodweb is referred to

as warmwater benthic. The base of the other version of the warmwater foodweb is primarily pelagic species (e.g., zooplankton) and is referred to as warmwater pelagic. Ideally, a location or State-specific foodweb would be calibrated to measured data. However, these hypothetical foodwebs are presented to evaluate the potential effect of alternate foodweb parameters on calculated FCMs and resulting HHWQC.

When the Gobas model is parameterized with assumptions and values representative of alternative warmwater hypothetical foodwebs rather than a Great Lakes foodweb, and a water temperature and sediment-water ratio more representative of warm surface waters but still assuming no metabolic transformation, the calculated FCMs for two of the three example chemicals increase for TL3 and decrease for TL4 (Table 8). Note that all of the hypothetical warmwater FCMs are substantially lower than the national FCMs developed by USEPA using assumptions and values representative of surface water and foodwebs of the Great Lakes. While the hypothetical warmwater foodwebs and associated FCMs are presented herein purely for illustrative purposes, the results indicate that developing a foodweb structure representative of state-specific lakes and streams in other locations throughout the United States has the potential to substantially alter the calculated FCMs.

Tables 8 and 12 show the resulting FCMs and national BAFs, respectively, for the three example chemicals (benzo(a)pyrene, fluoranthene, and dieldrin) from alternative model parameters and foodweb models. The differences can be quite large. For example, for BaP USEPA's national BAF is 3,900 L/kg based on the Great Lakes foodweb and no metabolism (Table 12). Simply accounting for metabolism, which is well known to occur, the BAF drops by more than four-fold to 900 L/kg, even assuming a Great Lakes foodweb (Table 12). In a warmwater benthic foodweb with a sediment-water ratio of 2 (representative of limited historical contamination), the BAF decreases to 400 L/kg, or nearly 10 times lower than USEPA's national BAF based on default assumptions (Table 12). In a warmwater pelagic food web with a sediment-water ratio of 2, the BAF is 500 L/kg, or nearly eight times lower than USEPA's default (Table 12). These relatively large decreases in BAF result in relatively large increases in HHWQC (Table 13).

In summary, the national default assumptions used by USEPA to derive FCMs are unlikely to be representative of conditions in all areas of the United States. USEPA's model is based on and calibrated for a Great Lakes foodweb using PCB data. As indicated above, hypothetical warm-water foodwebs will have substantially different inputs and structure and could result in different FCMs. In addition, assumptions of sediment contamination are based on areas that have a high historic loading followed by substantial reduction (e.g., PCBs in the Hudson River). USEPA's assumption for sediment-water ratio, the parameter that apportions the concentrations between sediment and the water column, is therefore higher than what would be expected in most waters of the United States resulting in larger FCMs than are likely representative of most United States surface waters. The sediment-water ratio has the most substantial effect on FCMs of the four model parameters varied in this report (Table 7). Finally, the temperature used in the USEPA model is cooler than might be expected in many United States waters. However, if metabolic transformation is not accounted for, an increase in temperature tends to increase FCMs because the higher temperature results in an increase in dietary intake in the model. This increased dietary intake is not balanced by what one might expect to be an increased rate of metabolism given that metabolism is assumed to be zero in USEPA's FCM model.

5 DERIVATION AND APPLICATION OF REFINED FCMS

The previous section reviewed in some detail the process used to derive FCMs and BAFs for the three example compounds. Finding the appropriate inputs to run the model USEPA used to derive FCMs and then to find and run the model to derive alternative FCMs can require substantial resources. Such resources may not be available to regulators charged with establishing State-specific HHWQC even though those same regulators know that the default assumptions used by USEPA to derive FCMs and BAFs are not representative of their State's waters or of the chemicals for which they are updating HHWQC. To assist such regulators in deriving more representative and applicable BAFs, this section describes the basis of alternative sets of FCMs derived to represent sets of conditions that differ from the single set of default conditions used by USEPA to derive the single set of FCMs it used when deriving BAFs to establish national HHWQC.

As with the table of default FCMs developed by USEPA, the alternative sets of FCMs are presented for a range of log K_{ow} (from 3 to 9) and for three trophic levels (TL2, TL3, and TL4). Seventy-two sets of alternative FCMs are presented (Appendix A). These correspond to different combinations of foodwebs, surface water temperature, sediment-water ratio, and metabolic transformation rate. The range of each assumption is described below followed by a brief description of the effect of some of the alternative assumptions (or combinations of assumptions) on FCMs (and resulting BAFs). This section concludes by describing how a State can easily use the alternative FCMs to refine the BAFs used by USEPA and develop BAFs and HHWQC that are more State-specific than USEPA's national defaults.

5.1 Foodweb

FCMs are presented for three different foodwebs. The first is the Lake Ontario foodweb used by USEPA to derive its default FCMs. As described above in Section 4.1.6, a foodweb comprised of warmwater species was also developed. FCMs are developed for two versions of the foodweb: a warmwater benthic foodweb in which the base of the foodweb is primarily benthic species (e.g., crayfish) and a second version in which the base of the foodweb is primarily pelagic species (e.g., zooplankton). The former foodweb is referred to as warmwater benthic and the latter as warmwater pelagic. The goal of providing FCMs for three foodwebs is to allow interested States and stakeholders to derive BAFs and HHWQC based on foodwebs that are more representative of surface waters in their states than Lake Ontario, the water body on which USEPA's BAFs and HHWQC are based.

5.2 Surface Water Temperature

Within each foodweb, FCMs are presented for two temperatures, 8° and 16°C. Eight degrees C is the temperature USEPA uses to derive its default FCMs and is intended to represent Lake Ontario. Because many surface waters throughout the United States are warmer than Lake Ontario, FCMs were also developed assuming a surface water temperature of 16°C, with the goal of allowing interested States and stakeholders to derive BAFs and HHWQC based on a temperature that is representative of surface waters in their states.

5.3 Sediment-Water Ratio

Within each foodweb and for each of the two temperatures, FCMs are presented for three sediment-water ratios: 23, 10, and 2. USEPA used a value of 23 to represent the ratio for compounds like PCBs in Lake Ontario. As described above, USEPA (2003) reports a range of ratios for waters with a history of high chemical loading and acknowledges that waters without such loading may have substantially lower ratios. Indeed, lower ratios may be the norm for most United States surface waters and waters with high historic chemical loading and relatively high ratios (e.g., Fox River and Green Bay, Lake Ontario, Hudson River) may be the exception. Ratios of 10 and 2 are used to develop FCMs to allow interested States and stakeholders to derive BAFs and HHWQC based on a sediment-water ratio that is representative of surface waters in their states.

5.4 Metabolic Transformation Rate Constant

Within each foodweb, for each of the four temperatures and for each of the three sediment water column quotients, FCMs are presented for three metabolic transformation rate constants: 0, 0.001, 0.01, and 0.1 (day^{-1}). USEPA assumed no metabolic transformation (i.e., a metabolic transformation rate constant of 0) when deriving default FCMs used to derive national BAFs. Most compounds undergo at least some metabolic transformation (Arnot et al. 2008). For some compounds the transformation is substantial. To allow States and interested stakeholders to derive BAFs and HHWQC that better represent the potential metabolism of chemicals, FCMs are presented that are based on four different metabolic transformation rate constants (i.e., 0. 0.001, 0.01, and 0.1 [day^{-1}]).

5.5 Effect of Varying FCM Parameters

Of the four parameters that are varied to refine FCMs and BAFs, the sediment-water ratio and metabolic transformation rate constant have the largest effect on FCMs and BAFs.

Decreasing the sediment-water ratio decreases trophic level-specific FCMs. This occurs because the base of all of the foodwebs includes benthic organisms. A high sediment-water ratio indicates that a large portion of the mass of a chemical in a surface water resides in sediments and not the water column. In such a case, sediments contribute the majority of a chemical to the foodweb. This is particularly true of the cold water and warmwater benthic foodwebs in which benthic and not pelagic organisms make up most of the base of the foodweb. As the sediment-water ratio decreases, the portion of a chemical in sediment decreases and the portion in the water column increases. This leads to less of the chemical entering the foodweb and that in turn leads to a decrease in the FCM. The decrease in FCM with decreasing sediment-water ratio is less pronounced in the warmwater pelagic foodweb because in that foodweb pelagic organisms make up a larger portion of the base of the foodweb than do benthic organisms. Decreases in the sediment-water ratio increase the mass of a chemical in the water column making more of the chemical available to pelagic organisms and the remainder of the foodweb.

Increasing the metabolic transformation rate constant leads to a decrease in the FCM. The decrease in FCM is expected because increased metabolism results in removal of a chemical from the foodweb leaving less of the chemical to be accumulated by higher trophic levels. In fact, when metabolic transformation is accounted for, FCMs can be less than 1.0 (see FCM summary tables that include a non-zero metabolic transformation rate constant in Appendix A). In developing its national trophic level-

specific FCMs, USEPA assumed no metabolic transformation thereby restricting the lowest FCM to a value of 1.0. For chemicals that undergo substantial metabolic transformation, FCMs, particularly for TL4, can be substantially less than 1.0 (see FCM tables that include a metabolic transformation rate constant of 1.0 in Appendix A).

Changing temperature or foodweb has a limited effect on FCMs. It is worth noting that temperature and metabolic transformation rate constant can interact such that refined FCMs can be larger than those based on USEPA's default assumptions. The interaction can occur if temperature is assumed to be higher than USEPA's default of 8°C and the metabolic transformation rate constant is assumed to be zero (i.e., metabolic transformation is assumed to not occur). In such cases the increased temperature results in increased uptake of a chemical by aquatic biota but without a corresponding increase in metabolism. For compounds that are metabolized, the increase uptake with increased temperature is "balanced" by increased metabolism as both uptake and metabolism (depuration) are biological processes affected by temperature.

5.6 Process for Refining FCMs, BAFs, and HHWQC

The process of refining the FCM, national BAF and ultimately the HHWQC to better represent conditions in the surface waters of a State than are represented by USEPA's default FCMs and national BAFs is relatively straightforward given the information summarized in Table 1 and the alternative FCMs presented in Appendix A. Table 1 presents the log K_{ow}, national BAF derivation method, the trophic level-specific national BAFs for TL2, TL3, and TL4, and the default FCMs USEPA used to derive the trophic level-specific national BAFs. National trophic level-specific BAFs can be refined and made more applicable to a specific State's surface waters, or to account for metabolism of a specific compound, by following the steps described below. (Note that this refinement is only applicable to national trophic level-specific BAFs derived using FCMs.)

1. Divide the default national trophic level-specific BAF by the default trophic level-specific FCM USEPA used to derive the national trophic level-specific BAF.
2. Select from Tables 2-73 in Appendix A, a trophic level-specific FCM that better represents a State's surface waters, or a chemical's metabolic transformation, or both;
3. Multiply the BAF that resulted from Step 1 above by the trophic level-specific FCM selected in Step 2. The resulting BAF is a State (and/or chemical)-specific and trophic level-specific BAF.
4. Recalculate USEPA's national HHWQC using the State-specific BAF for that chemical.

A hypothetic application of this methodology is presented below for chlordane[7]. The national trophic level-specific BAFs for chlordane of 5,300, 44,000, and 60,000 for TL2, TL3, and TL4, respectively (Table 1), are derived using the log K_{ow}*FCM method and national trophic level-specific FCMs of 1, 6.15, and 7.194 for TL2, TL3, and TL4, respectively (Table 1). Dividing each of the trophic level-specific BAFs by the trophic level-specific FCMs results in trophic level-specific BAFs (unadjusted for accumulation from the foodweb or metabolism) of 5,300, 7,154, and 8,340 for TL2, TL3, and TL4, respectively. (Note that the

[7] While this methodology could have been applied to one of the example chemicals described in Sections 3 and 4 (benzo(a)pyrene, fluoranthene, and dieldrin), alternative FCMs, BAFs and HHWQC using chemical-specific K_{ow}s and K_ms have already been derived and presented in Section 4. Thus, chlordane was selected to illustrate another example of how local conditions might be reflected in BAF estimates.

resulting unadjusted BAFs are not all identical because the national trophic level-specific BAFs included trophic level-specific differences in assumed lipid content of fish and shellfish.)

For this example, assume that the HHWQC are being a developed by a State with warm waters (relative to the Great Lakes temperature assumption of 8ºC) dominated by benthic foodwebs, no history of historical loading of chlordane, and that we have no information on metabolic transformation rates for chlordane. In such a case, a more representative FCM can be found on Table 31 of Appendix A. That table presents FCMs for warmwater benthic foodwebs, with an annual temperature of 16°C, a sediment-water ratio of 2 and no metabolic transformation. USEPA reports that chlordane has a log K_{ow} of 5.54. The trophic level-specific FCMs at log K_{ow} of 5.5 shown on Table 31 are 1, 1.64, and 1.99 and at log K_{ow} of 5.6 are 1, 1.74, and 2.17 for TL2, TL3, and TL4, respectively. Using linear interpolation, refined trophic level-specific FCMs of 1, 1.68, and 2.06 can be derived for TL2, TL3, and TL4, respectively. Multiplying the unadjusted trophic level-specific BAFs from Step 1 by the refined trophic level-specific FCMs results in refined trophic level-specific BAFs for chlordane of 5,300, 12,020, and 17,180 (L/kg) for TL2, TL3, and TL4, respectively. For TL2 the refined BAF and the national BAF are identical, but for TL3 and TL4 the refined trophic level-specific BAFs are three times and five times, respectively, lower than the corresponding national trophic level-specific BAFs. That in turn leads to a refined HHWQC for organisms and water of 0.00098 ug/L and for consumption of organisms only of 0.00099 ug/L, compared to national recommended HHWQC derived by USEPA using default FCMs of 0.00031 and 0.00032 ug/L, respectively.

The above example does not include metabolic transformation. The differences between HHWQC based on default and refined BAFs can be even larger when metabolism is accounted for. To provide a sense of the change in HHWQC using different combinations of assumptions, Table 13 and Figures 2 and 3 present alternative HHWQC for the BaP and dieldrin (the two example chemicals discussed above for which USEPA used FCMs to estimate national BAFs). For these two chemicals, HHWQC can vary by up to 10-fold. The one set of assumptions that generally leads to HHWQC that are lower than USEPA's national HHWQC uses all of USEPA's defaults except temperature, which is changed from 8 to 16°C. That change increases uptake of a chemical without a corresponding increase in metabolic transformation. However, all the refined scenarios presented in Table 13 and Figures 2 and 3 include chemical specific metabolic transformation and as a result all the refined HHWQC are higher than USEPA's national HHWQC.

USEPA (2016) describes modifications to the national BAF based on State-specific lipid fraction of fish and shellfish and DOC and POC concentrations in ambient water. When Florida made those two adjustments, Florida-specific HHWQC increased because Florida-specific DOC and POC concentrations were higher than the national defaults and Florida-specific lipid fractions were lower than national defaults (FDEP 2016). The magnitude of the decrease varied between chemicals because the freely dissolved concentration depends on the K_{ow} of a chemical as well as the DOC and POC concentration. Whether a similar increase occurs in other States when local lipid content and DOC and POC concentrations are used will depend on how the State-specific concentrations compare to USEPA's national defaults. It is unlikely that State-specific lipid and DOC and POC concentrations will have an effect on HHWQC as large as the effect of some of the assumptions used to derive alternative FCMs.

As summarized in Arcadis (2018), other assumptions and aspects of the method used by USEPA to derive national trophic level-specific BAFs can also be refined. One example is USEPA's assumption that laboratory water used to estimate BCFs had a DOC and POC concentration equal to the median of the

DOC and POC concentration in ambient United States surface water for laboratory studies that did not report DOC and POC concentrations. However, many laboratories use filtered water. Filtered water has lower concentrations of DOC and POC than ambient water. The effect of accounting for filtration of laboratory water is to increase the dissolved concentration of a chemical in the laboratory study. That in turn decreases the BCF, which leads to a lower national BAF and a higher HHWQC. That effect too, however, is relatively small compared to the changes in HHWQC based on changes to assumptions used to derive FCMs.

In summary, the information presented above makes clear that alternative FCMs and BAFs are likely to be more representative of many surface waters in the United States than USEPA's default FCMs and national BAFs. Further, the differences between USEPA's national BAFs and the refined BAFs can be substantial leading to similarly substantial changes in HHWQC. Lastly, the alternative FCMs provided in Appendix A combined with information summarized in Table 1 and the straightforward procedure described in this section can be used by States and interested stakeholders to develop refined State- and chemical-specific, FCMs, BAFs and HHWQC.

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TABLES

Table 1 - Summary of Chemical Characteristics, Methods, and Parameters used by USEPA for the Derivation of HHWQCs for 94 Chemicals

CAS Number	Chemical Name	Mean Log K_{ow}	Method (for baseline BAF/BCF)	Foodchain Multiplier			National BAF/BCF (L/kg-tissue)		
				TL2	TL3	TL4	TL2	TL3	TL4
107-13-1	Acrylonitrile	-0.92	Log K_{ow}	--	--	--	1	1	1
542-88-1	Bis(Chloromethyl)Ether	-0.38	Log K_{ow}	--	--	--	1	1	1
107-02-8	Acrolein	-0.01	Log K_{ow}	--	--	--	1	1	1
57-12-5	Cyanide	0.87	2003 BCF	--	--	--	1	1	1
74-83-9	Methyl Bromide	1.1	Log K_{ow}	--	--	--	1.2	1.3	1.4
75-09-2	Methylene Chloride	1.3	Log K_{ow}	--	--	--	1	2	2
92-87-5	Benzidine	1.34	Log K_{ow}	--	--	--	1.4	1.6	1.7
111-44-4	Bis(2-Chloroethyl) Ether	1.34	Log K_{ow}	--	--	--	1.4	1.6	1.7
75-01-4	Vinyl Chloride	1.36	Log K_{ow}	--	--	--	1.4	1.6	1.7
108-95-2	Phenol	1.46	Log K_{ow}	--	--	--	1.5	1.7	1.9
107-06-2	1,2-Dichloroethane	1.48	Log K_{ow}	--	--	--	1.6	1.8	1.9
51-28-5	2,4-Dinitrophenol	1.54	Alternative BAF[a]	--	--	--	4.4	4.4	4.4
25550-58-7	Dinitrophenols	1.55	2002 BCF	--	--	--	1.51	1.51	1.51
131-11-3	Dimethyl Phthalate	1.6	Alternative BAF[b]	--	--	--	4,000	4,000	4,000
78-59-1	Isophorone	1.67	Log K_{ow}	--	--	--	1.9	2.2	2.4
75-35-4	1,1-Dichloroethylene	1.73	Log K_{ow}	--	--	--	2	2.4	2.6
542-75-6	1,3-Dichloropropene	1.82	Log K_{ow}	--	--	--	2.3	2.7	3
98-95-3	Nitrobenzene	1.84	Log K_{ow}	--	--	--	2.3	2.8	3.1
67-66-3	Chloroform	1.97	Log K_{ow}	--	--	--	2.8	3.4	3.8
121-14-2	2,4-Dinitrotoluene	1.98	Log K_{ow}	--	--	--	2.8	3.5	3.9
78-87-5	1,2-Dichloropropane	1.99	Log K_{ow}	--	--	--	2.9	3.5	3.9
156-60-5	1,2-Trans-Dichloroethylene	2.09	Log K_{ow}	--	--	--	3.3	4.2	4.7
75-27-4	Dichlorobromomethane	2.10	Log K_{ow}	--	--	--	3.4	4.3	4.8
71-43-2	Benzene	2.13	Log K_{ow}	--	--	--	3.6	4.5	5
124-48-1	Chlorodibromomethane	2.16	Log K_{ow}	--	--	--	3.7	4.8	5.3
95-57-8	2-Chlorophenol	2.17	Log K_{ow}	--	--	--	3.8	4.8	5.4
105-67-9	2,4-Dimethylphenol	2.3	Log K_{ow}	--	--	--	5	6.2	7
84-66-2	Diethyl Phthalate	2.35	Alternative BAF[b]	--	--	--	920	920	920
79-34-5	1,1,2,2-Tetrachloroethane	2.39	Log K_{ow}	--	--	--	5.7	7.4	8.4
75-25-2	Bromoform	2.4	Log K_{ow}	--	--	--	5.8	7.5	8.5
79-00-5	1,1,2-Trichloroethane	2.42	Log K_{ow}	--	--	--	6	7.8	8.9
108-60-1	Bis(2-Chloro-1-Methylethyl) Ether	2.48	Log K_{ow}	--	--	--	7	8.8	10
534-52-1	2-Methyl-4,6-Dinitrophenol	2.49	Log K_{ow}	--	--	--	6.8	8.9	10
71-55-6	1,1,1-Trichloroethane	2.49	Log K_{ow}	--	--	--	6.9	9	10
79-01-6	Trichloroethylene	2.61	Log K_{ow}	--	--	--	8.7	12	13
56-23-5	Carbon Tetrachloride	2.64	Log K_{ow}	--	--	--	9.3	12	14
108-88-3	Toluene	2.72	Log K_{ow}	--	--	--	11	15	17
94-75-7	Chlorophenoxy Herbicide (2,4-D)	2.81	Alternative BAF[c]	--	--	--	58	58	58
108-90-7	Chlorobenzene	2.84	Log K_{ow}	--	--	--	14	19	22
122-66-7	1,2-Diphenylhydrazine	2.94	Log K_{ow}	--	--	--	18	24	27
59-50-7	3-Methyl-4-Chlorophenol	3.1	Log K_{ow}	--	--	--	25	34	39
120-83-2	2,4-Dichlorophenol	3.2	Log K_{ow}	--	--	--	31	42	48

Table 1 - Summary of Chemical Characteristics, Methods, and Parameters used by USEPA for the Derivation of HHWQCs for 94 Chemicals

CAS Number	Chemical Name	Mean Log K_{ow}	Method (for baseline BAF/BCF)	Foodchain Multiplier			National BAF/BCF (L/kg-tissue)		
				TL2	TL3	TL4	TL2	TL3	TL4
91-94-1	3,3'-Dichlorobenzidine	3.36	Log K_{ow}	--	--	--	44	60	69
127-18-4	Tetrachloroethylene	3.4	Log K_{ow}	--	--	--	49	66	76
95-50-1	1,2-Dichlorobenzene	3.43	Log K_{ow}	--	--	--	52	71	82
106-46-7	1,4-Dichlorobenzene	3.44	BCF	--	--	--	28	66	84
541-73-1	1,3-Dichlorobenzene	3.53	BCF	--	--	--	31	120	190
67-72-1	Hexachloroethane	3.58	Field BAFs	--	--	--	1,200	280	600
33213-65-9	beta-Endosulfan	3.62	Log K_{ow}	--	--	--	80	110	130
1031-07-8	Endosulfan Sulfate	3.66	Log K_{ow}	--	--	--	88	120	140
88-06-2	2,4,6-Trichlorophenol	3.69	Log K_{ow}	--	--	--	94	130	150
95-95-4	2,4,5-Trichlorophenol	3.72	Log K_{ow}	--	--	--	100	140	160
58-89-9	gamma-BHC (Lindane)	3.72	Field BAFs	--	--	--	1,200	2,400	2,500
100-41-4	Ethylbenzene	3.74	Log K_{ow}	--	--	--	100	140	160
319-85-7	beta-BHC	3.78	Log K_{ow}	--	--	--	110	160	180
93-72-1	Chlorophenoxy Herbicide (2, 4, 5-TP)	3.8	Alternative BAF[a]	--	--	--	13	13	13
319-84-6	alpha-Hexachlorocyclohexane (HCH)	3.8	Field BAF	--	--	--	1,700	1,400	1,500
959-98-8	alpha-Endosulfan	3.83	Log K_{ow}	--	--	--	130	180	200
91-58-7	2-Chloronaphthalene	3.9	Log K_{ow}	--	--	--	150	210	240
608-73-1	Hexachlorocyclohexane	3.93	Log K_{ow}	--	--	--	160	220	250
83-32-9	Acenaphthene	3.98	BCF	--	--	--	510	510	510
120-82-1	1,2,4-Trichlorobenzene	4.02	Field BAF	--	--	--	2,800	1,500	430
86-73-7	Fluorene	4.18	BCF	--	--	--	230	450	710
84-74-2	Di-n-Butyl Phthalate	4.21	Field BAF[b]	--	--	--	2,900	2,900	2,900
7421-93-4	Endrin Aldehyde	4.373	Field BAF	--	--	--	440	920	850
120-12-7	Anthracene	4.45	BCF	--	--	--	610	610	610
77-47-4	Hexachlorocyclopentadiene	4.52	Log K_{ow}*FCM	1	1.734	1.344	620	1,500	1,300
95-94-3	1,2,4,5-Tetrachlorobenzene	4.6	Field BAF	--	--	--	17,000	2,900	1,500
85-68-7	Butylbenzyl Phthalate	4.73	Field BAF[b]	--	--	--	19,000	19,000	19,000
87-68-3	Hexachlorobutadiene	4.78	Field BAF	--	--	--	23,000	2,800	1,100
129-00-0	Pyrene	4.88	BCF[a]	--	--	--	860	860	860
72-43-5	Methoxychlor	4.88	Log K_{ow}*FCM	1	2.578	2.06	1,400	4,800	4,400
206-44-0	Fluoranthene	4.9	BCF	--	--	--	1,500	1,500	1,500
8001-35-2	Toxaphene	4.97	Log K_{ow}*FCM	1	2.892	2.393	1,700	6,600	6,300
87-86-5	Pentachlorophenol	5.01	BCF*FCM	1	3.043	2.561	44	290	520
218-01-9	Chrysene	5.16	BCF*FCM[e]	1	10.216	15.98	3,900	3,900	3,900
608-93-5	Pentachlorobenzene	5.18	Field BAFs	--	--	--	3,500	4,500	10,000
1024-57-3	Heptachlor Epoxide	5.4	Log K_{ow}*FCM	1	5.14	5.48	4,000	28,000	35,000
72-20-8	Endrin	5.47	Log K_{ow}*FCM	1	5.637	6.299	4,600	36,000	46,000
57-74-9	Chlordane	5.54	Log K_{ow}*FCM	1	6.15	7.194	5,300	44,000	60,000
56-55-3	Benzo (a) Anthracene	5.61	BCF*FCM[e]	1	10.216	15.98	3,900	3,900	3,900
118-74-1	Hexachlorobenzene	5.73	Field BAF	--	--	--	18,000	46,000	90,000
72-54-8	4,4'-DDD	6.02	Field BAF	--	--	--	33,000	140,000	240,000
205-99-2	Benzo (b) Fluoranthene	6.04	BCF*FCM[e]	1	10.216	15.98	3,900	3,900	3,900
50-32-8	Benzo (a) Pyrene	6.06	BCF*FCM[b,d]	1	10.216	15.98	3,900	3,900	3,900
207-08-9	Benzo (k) Fluoranthene	6.06	BCF*FCM[e]	1	10.216	15.98	3,900	3,900	3,900

Table 1 - Summary of Chemical Characteristics, Methods, and Parameters used by USEPA for the Derivation of HHWQCs for 94 Chemicals

CAS Number	Chemical Name	Mean Log K_{ow}	Method (for baseline BAF/BCF)	Foodchain Multiplier			National BAF/BCF (L/kg-tissue)		
				TL2	TL3	TL4	TL2	TL3	TL4
76-44-8	Heptachlor	6.1	Log K_{ow}*FCM	1	10.5	16.7	12,000	180,000	330,000
60-57-1	Dieldrin	6.2	Log K_{ow}*FCM	1	11.2	18.5	14,000	210,000	410,000
309-00-2	Aldrin	6.5	Log K_{ow}*FCM	1	12.6	22.8	18,000	310,000	650,000
72-55-9	4,4'-DDE	6.51	Field BAFs	--	--	--	270,000	1,100,000	3,100,000
193-39-5	Indeno (1,2,3-cd) Pyrene	6.58	BCF*FCM[e]	1	10.216	15.98	3,900	3,900	3,900
53-70-3	Dibenzo (a,h) Anthracene	6.84	BCF*FCM[e]	1	10.216	15.98	3,900	3,900	3,900
50-29-3	4,4'-DDT	6.91	Field BAF	--	--	--	35,000	240,000	1,100,000
117-81-7	Bis(2-Ethylhexyl) Phthalate	7.5	Field BAF[b]	--	--	--	710	710	710

[a]geometric mean of the TL2 and TL3 BCFs
[b]geometric mean of the TL3 and TL4 BAFs
[c]BCF method estimate with the BCF value availabel for 2,4,5-TP
[d]USEPA procedure calls for BCF method but USEPA used BCF*FCM method
[e]Benzo(a)Pyrene BAFs used to represent this PAH

Notes
BAF = Bioaccumulation factor
BCF = Bioconcentration factor
FCM = Food chain multiplier
-- = FCM not used in the derivation of BAF values for chemicals with Kow < 4 or if ≥ 4 and known to have high metabolism
HHWQC = human health water quality criteria
K_{ow} = n-octanol-water partition coefficient

Table 2 - USEPA Published Foodchain Multipliers (from USEPA (2003), Table 4-6, p 4-39)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
4.0	1.00	1.23	1.07
4.1	1.00	1.29	1.09
4.2	1.00	1.36	1.13
4.3	1.00	1.45	1.17
4.4	1.00	1.56	1.23
4.5	1.00	1.70	1.32
4.6	1.00	1.87	1.44
4.7	1.00	2.08	1.60
4.8	1.00	2.33	1.82
4.9	1.00	2.64	2.12
5.0	1.00	3.00	2.51
5.1	1.00	3.43	3.02
5.2	1.00	3.93	3.68
5.3	1.00	4.50	4.49
5.4	1.00	5.14	5.48
5.5	1.00	5.85	6.65
5.6	1.00	6.60	8.01
5.7	1.00	7.40	9.54
5.8	1.00	8.21	11.20
5.9	1.00	9.01	13.00
6.0	1.00	9.79	14.90
6.1	1.00	10.50	16.70
6.2	1.00	11.20	18.50
6.3	1.00	11.70	20.10
6.4	1.00	12.20	21.60
6.5	1.00	12.60	22.80
6.6	1.00	12.90	23.80
6.7	1.00	13.20	24.40
6.8	1.00	13.30	24.70
6.9	1.00	13.30	24.70
7.0	1.00	13.20	24.30
7.1	1.00	13.10	23.60
7.2	1.00	12.80	22.50
7.3	1.00	12.50	21.20
7.4	1.00	12.00	19.50
7.5	1.00	11.50	17.60
7.6	1.00	10.80	15.50
7.7	1.00	10.10	13.30
7.8	1.00	9.31	11.20
7.9	1.00	8.46	9.11
8.0	1.00	7.60	7.23
8.1	1.00	6.73	5.58
8.2	1.00	5.88	4.19
8.3	1.00	5.07	3.07
8.4	1.00	4.33	2.20
8.5	1.00	3.65	1.54
8.6	1.00	3.05	1.06
8.7	1.00	2.52	0.72
8.8	1.00	2.08	0.48
8.9	1.00	1.70	0.32
9.0	1.00	1.38	0.21

Notes

K_{ow} = n-octanol-water partition coefficient

Reference

USEPA. 2003. Methodology for Deriving Ambient Water Quality Criteria for the Protection of Human Health (2000). Technical Support Document Volume 2: Development of National Bioaccumulation Factors. EPA-822-R-03-030

Table 3a - USEPA Calculation of Baseline BAFs by Trophic Level using the BCF Method for Benzo(a)pyrene

Reference	Species	BCF (L/kg-tissue)	Trophic Level (TL)	Foodchain Multiplier TL 2	Foodchain Multiplier TL 3	Foodchain Multiplier TL 4	Fraction Freely Dissolved (f_{fd})	Selected Lipid Fraction (f_ℓ)	Baseline BAF (L/kg-lipid) =FCM*(BAF/f_{fd}-1)/f_ℓ	Geomeans Calculated by Species	Geomeans Calculated by Trophic Level
Landrum and Poore 1988	Amphipod	40,275	2	1	10.216	15.98	0.5433	0.03	2,470,769	2,470,769	
Landrum and Poore 1988	Mayfly	5,870	2	1	10.216	15.98	0.5433	0.03	360,081	360,081	
Landrum and Poore 1988	Shrimp	7,466	2	1	10.216	15.98	0.5433	0.017	808,223	808,223	
McCarthy 1983	Water flea	8,000	2	1	10.216	15.98	0.5433	0.05	294,452	294,452	
Gossiaux et al 1996	Zebra mussel	24,000	2	1	10.216	15.98	0.5433	0.13	339,767		
Gossiaux et al 1996	Zebra mussel	40,000	2	1	10.216	15.98	0.5433	0.1	736,169		
Gossiaux et al 1996	Zebra mussel	49,000	2	1	10.216	15.98	0.5433	0.08	1,127,262		
Gossiaux et al 1996	Zebra mussel	61,000	2	1	10.216	15.98	0.5433	0.0925	1,213,690		
Gossiaux et al 1996	Zebra mussel	62,000	2	1	10.216	15.98	0.5433	0.0925	1,233,587		
Gossiaux et al 1996	Zebra mussel	77,000	2	1	10.216	15.98	0.5433	0.09	1,574,595		
Gossiaux et al 1996	Zebra mussel	83,000	2	1	10.216	15.98	0.5433	0.0925	1,651,419		
Gossiaux et al 1996	Zebra mussel	107,000	2	1	10.216	15.98	0.5433	0.0925	2,128,940		862,368
Gossiaux et al 1996	Zebra mussel	116,000	2	1	10.216	15.98	0.5433	0.07	3,049,872		
Gossiaux et al 1996	Zebra mussel	132,000	2	1	10.216	15.98	0.5433	0.15	1,619,588	2,252,602	
Gossiaux et al 1996	Zebra mussel	147,000	2	1	10.216	15.98	0.5433	0.1	2,705,449		
Gossiaux et al 1996	Zebra mussel	150,000	2	1	10.216	15.98	0.5433	0.07	3,943,804		
Gossiaux et al 1996	Zebra mussel	165,000	2	1	10.216	15.98	0.5433	0.07	4,338,186		
Gossiaux et al 1996	Zebra mussel	167,000	2	1	10.216	15.98	0.5433	0.0925	3,322,745		
Gossiaux et al 1996	Zebra mussel	191,000	2	1	10.216	15.98	0.5433	0.08	4,394,058		
Gossiaux et al 1996	Zebra mussel	197,000	2	1	10.216	15.98	0.5433	0.07	5,179,533		
Gossiaux et al 1996	Zebra mussel	215,000	2	1	10.216	15.98	0.5433	0.1	3,956,954		
Gossiaux et al 1996	Zebra mussel	220,000	2	1	10.216	15.98	0.5433	0.07	5,784,252		
Gossiaux et al 1996	Zebra mussel	273,000	2	1	10.216	15.98	0.5433	0.0925	5,431,799		
Jimenez et al 1987	Bluegill sunfish	377	3	1	10.216	15.98	0.5433	0.08366667	84,599		
Jimenez et al 1987	Bluegill sunfish	842	3	1	10.216	15.98	0.5433	0.08366667	189,106	120,798	120,798
Spacie et al 1983	Bluegill sunfish	490	3	1	10.216	15.98	0.5433	0.08366667	109,993		
Spacie et al 1983	Bluegill sunfish	539	3	1	10.216	15.98	0.5433	0.08366667	121,005		

Notes

FCM = foodchain multiplier

TL = trophic level

f_{fd} = fraction freely dissolved

f_ℓ = lipid fraction

BCF = bioconcentration factor

BAF = bioaccumulation factor

L = liter

kg = kilogram

geomean = geometric mean, defined as the nth root of the product of n numbers

Table 3b - USEPA Calculation of National BAF from Baseline BAF for Benzo(a)pyrene

Trophic Level	Baseline BAF by TL (L/kg-lipid)	National BAF (L/kg)[a] $=(BAF*f_{\ell}+1)*f_{fd}$	National BAF (L/kg) Rounded	Geomean of National BAF (L/kg) by TL
TL 2	862,368	8,848	8,900	3,900
TL 3	120,798	1,697	1,700	

[a] default national lipid fraction TL2 = 0.019, TL3 - 0.026; benzo(a)pyrene f_{fd} = 0.5433

Notes

TL = trophic level

f_{fd} = fraction freely dissolved

f_{ℓ} = lipid fraction

BAF = bioaccumulation factor

L = liter

kg = kilogram

geomean = geometric mean, defined as the nth root of the product of n numbers

Table 4a - USEPA Calculation of Baseline BAFs by Trophic Level using the BCF Method for Fluoranthene

Reference	Species	BCF (L/kg-tissue)	Trophic Level (TL)	Foodchain Multiplier TL 2	Foodchain Multiplier TL 3	Foodchain Multiplier TL 4	Fraction Freely Dissolved (f_{fd})	Selected Lipid Fraction (f_{ℓ})	Baseline BAF (L/kg-lipid) =FCM*(BAF/f_{fd}-1)/f_{ℓ}	Geomeans Calculated by Species
Sheedy et al 1998	Oligochaete	1510	2	1	2.64	2.12	0.945050219	0.03	53,227	80,714
Sheedy et al 1998	Oligochaete	2580	2	1	2.64	2.12	0.945050219	0.03	90,967	
Sheedy et al 1998	Oligochaete	3080	2	1	2.64	2.12	0.945050219	0.03	108,603	

Notes

FCM = foodchain multiplier
TL = trophic level
f_{fd} = fraction freely dissolved
f_{ℓ} = lipid fraction
BCF = bioconcentration factor
BAF = bioaccumulation factor
L = liter
kg = kilogram
geomean = geometric mean, defined as the nth root of the product of n numbers

Table 4b - USEPA Calculation of National BAF from Baseline BAF for Fluoranthene

Trophic Level	Baseline BAF by TL (L/kg-lipid)	National BAF[a] =(BAF*f_ℓ+1)*f_{fd}	National BAF (L/kg) Rounded
TL 2	80,714	1,450	1,500

[a] default national lipid fraction TL2 = 0.019; fluoranthene f_{fd} = 0.945050219

Notes

TL = trophic level

f_{fd} = fraction freely dissolved

f_ℓ = lipid fraction

BAF = bioaccumulation factor

L = liter

kg = kilogram

geomean = geometric mean, defined as the nth root of the product of n numbers

Table 5a - USEPA Calculation of Baseline BAFs by Trophic Level using the BAF Method for Di-n-Butyl Phthalate

Reference	Species	BAF (L/kg-tissue)	Trophic Level (TL)	Foodchain Multiplier TL 2	Foodchain Multiplier TL 3	Foodchain Multiplier TL 4	Fraction Freely Dissolved (f_{fd})	Selected Lipid Fraction (f_ℓ)	Baseline BAF (L/kg-lipid) =(BAF/f_{fd}-1)/f_ℓ	Geomeans Calculated by Species	Geomeans Calculated by Trophic Level
Gobas et al 2003	Pacific Staghorn Sculpin	1119.36057	4	1	1.369	1.134	0.988267633	0.003	377,216	377,216	74,484
Mackintosh 2002	Pacific Staghorn Sculpin	1119.36057	4	1	1.369	1.134	0.988267633	0.003	377,216		
Mackintosh 2002	Pile Perch	353.972892	4	1	1.369	1.134	0.988267633	0.007	51,025	51,025	
Gobas et al 2003	Spiny Dogfish	285.819108	4	1	1.369	1.134	0.988267633	0.083	3,472	1,998	
Mackintosh 2002	Spiny Dogfish	95.2730359	4	1	1.369	1.134	0.988267633	0.083	1,149		
Mackintosh 2002	Striped Seaperch	1345.7674	4	1	1.369	1.134	0.988267633	0.0017	800,438	800,438	
Mackintosh 2002	Whitespotted Greenling	587.448777	3	1	1.369	1.134	0.988267633	0.006	98,904	98,904	142,876
Mackintosh 2002	English Sole	1020.86897	3	1	1.369	1.134	0.988267633	0.005	206,398	206,398	

Notes
FCM = foodchain multiplier
TL = trophic level
f_{fd} = fraction freely dissolved
f_ℓ = lipid fraction
BCF = bioconcentration factor
BAF = bioaccumulation factor
L = liter
kg = kilogram
geomean = geometric mean, defined as the nth root of the product of n numbers

Table 5b - USEPA Calculation of National BAF from Baseline BAF for Di-n-Butyl Phthalate

Trophic Level	Baseline BAF by TL (L/kg-lipid)	National BAF (L/kg)[a] $=(BAF*f_{\ell}+1)*f_{fd}$	National BAF by TL (L/kg) Rounded	National BAF (L/kg) Rounded
TL3	142,876	3,672	3,700	2900
TL4	74,484	2,209	2,200	

[a] default national lipid fraction TL3 = 0.026 and TL4 = 0.03; di-n-butyl phthalate f_{fd} = 0.988267632645215

Notes

TL = trophic level

f_{fd} = fraction freely dissolved

f_{ℓ} = lipid fraction

BAF = bioaccumulation factor

L = liter

kg = kilogram

geomean = geometric mean, defined as the nth root of the product of n numbers

Table 6 - USEPA Calculation of Baseline BAFs by Trophic Level using the K_{ow} Method for Dieldrin

Trophic Level	K_{ow}	FCM	Baseline BAF (L/kg-lipid) =FCM*K_{ow}	Default National Lipid Fraction (f_ℓ)	Fraction Freely Dissolved (f_{fd})	National BAF (L/kg) =(BAF*f_ℓ+1)*f_{fd}	National BAF (L/kg) Rounded
2	1584893.19	1	1584893.192	0.019	0.462932569	13941	14000
3	1584893.19	11.2	17750803.76	0.026	0.462932569	213654	210000
4	1584893.19	18.5	29320524.06	0.03	0.462932569	407203	410000

Notes

FCM = foodchain multiplier

TL = trophic level

f_{fd} = fraction freely dissolved

f_ℓ = lipid fraction

BAF = bioaccumulation factor

L = liter

kg = kilogram

Table 7 - Summary of USEPA Model Input Parameters to the Gobas (1993) Model to Calculate Foodchain Multipliers and Alternative Model Inputs Evaluated in the Report

Model Parameter	Default USEPA value	Units	Range of values evaluated in this report
Water Temperature	8	° C	8; 16
Organic content of water	1.00E-30	kg/L	Not changed
Organic carbon content of sediment	2.70%	%	Not changed
Density of lipids	0.9	kg/L	Not changed
Density of organic carbon	0.9	kg/L	Not changed
$\Pi_{SOCW/Kow}$	23	--	23; 10; 2
K_m[a]	0	--	0; chemical-specific
Foodweb	Coldwater (Great Lakes)	--	Coldwater (Great Lakes); Warmwater - benthic; Warmwater - pelagic

[a]See Tables 9 and 10 for chemical-specific normalized K_ms evaluated in this report

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

-- = unitless

L = liter

kg = kilogram

References

Gobas, F.A.P. 1993. A Model for Predicting the Bioaccumulation Hydrophobic Organic Chemicals in Aquatic Food-webs: Application to Lake Ontario. Ecological Modelling, 69:1-17.

Table 8 - Foodchain Multipliers Resulting from Alternative Foodweb Model Scenarios

Foodweb	Metabolism (K_m)	Water Temperature (° C)	$\Pi_{SOCW/Kow}$	Benzo(a)pyrene			Fluoranthene			Dieldrin		
				TL 2	TL 3	TL 4	TL 2	TL 3	TL 4	TL 2	TL 3	TL 4
USEPA Default/Coldwater (Great Lakes)	0	8	23	1.00	10.32	15.80	1.00	2.64	2.10	1.00	11.29	18.35
Coldwater (Great Lakes)	Chemical-specific	8	23	1.00	0.30	0.02	1.00	0.29	0.05	1.00	6.31	5.74
Coldwater (Great Lakes)	Chemical-specific	8	10	1.00	0.15	0.01	1.00	0.19	0.05	1.00	3.03	2.88
Coldwater (Great Lakes)	Chemical-specific	8	2	1.00	0.05	0.01	1.00	0.12	0.05	1.00	0.99	1.12
Coldwater (Great Lakes)	Chemical-specific	16	23	1.00	0.44	0.03	1.00	0.32	0.06	1.00	8.37	10.05
Coldwater (Great Lakes)	Chemical-specific	16	10	1.00	0.21	0.02	1.00	0.19	0.05	1.00	3.98	4.94
Coldwater (Great Lakes)	Chemical-specific	16	2	1.00	0.07	0.01	1.00	0.11	0.04	1.00	1.24	1.79
Warmwater - benthic	0	8	23	1.00	11.20	13.84	1.00	2.56	2.18	1.00	12.49	15.87
Warmwater - benthic	Chemical-specific	8	23	1.00	0.45	0.10	1.00	0.50	0.15	1.00	7.93	6.81
Warmwater - benthic	Chemical-specific	8	10	1.00	0.22	0.05	1.00	0.33	0.11	1.00	3.80	3.25
Warmwater - benthic	Chemical-specific	8	2	1.00	0.08	0.02	1.00	0.22	0.08	1.00	1.25	0.78
Warmwater - benthic	Chemical-specific	16	23	1.00	0.66	0.15	1.00	0.65	0.18	1.00	10.44	10.73
Warmwater - benthic	Chemical-specific	16	10	1.00	0.31	0.07	1.00	0.39	0.12	1.00	4.94	5.05
Warmwater - benthic	Chemical-specific	16	2	1.00	0.10	0.02	1.00	0.23	0.08	1.00	1.56	1.14
Warmwater - pelagic	0	8	23	1.00	5.20	7.59	1.00	1.64	1.88	1.00	5.73	8.48
Warmwater - pelagic	Chemical-specific	8	23	1.00	0.21	0.09	1.00	0.32	0.14	1.00	3.64	3.88
Warmwater - pelagic	Chemical-specific	8	10	1.00	0.15	0.04	1.00	0.28	0.10	1.00	2.61	2.43
Warmwater - pelagic	Chemical-specific	8	2	1.00	0.12	0.02	1.00	0.25	0.08	1.00	1.97	1.15
Warmwater - pelagic	Chemical-specific	16	23	1.00	0.30	0.13	1.00	0.38	0.17	1.00	4.73	5.80
Warmwater - pelagic	Chemical-specific	16	10	1.00	0.21	0.06	1.00	0.32	0.12	1.00	3.36	3.68
Warmwater - pelagic	Chemical-specific	16	2	1.00	0.16	0.02	1.00	0.28	0.08	1.00	2.51	1.75

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

TL = trophic level

Table 9 - Summary of Chemical-specific Metabolic Transformation Rate Constants (K_m) Used in the Gobas (1993) Model to Calculate Alternative Foodchain Multipliers for Three Chemicals

Chemical	Log K_m[a] [Arnot et al (2008)]	Study Species	Reference [from Arnot et al (2008)]
Benzo(a)pyrene	0.04	Rainbow trout	Niimi, AJ and V Palazzo. 1986. Wat. Res. 20(4):503-507
Benzo(a)pyrene	-0.46	Rainbow trout	http://www.hesiglobal.org/Committees/ProjectCommittees/Bioaccumulation/
Benzo(a)pyrene	-0.20	Bluegill sunfish	Spacie, A., P. F. Landrum, and G. J. Leversee. 1983. Ecotox. Env. Saf. 7:330-341
Fluoranthene	-0.46	Rainbow trout	Niimi, AJ and V Palazzo. 1986. Wat. Res. 20(4):503-507
Fluoranthene	0.05	Rainbow trout	http://www.hesiglobal.org/Committees/ProjectCommittees/Bioaccumulation/
Fluoranthene	-0.02	Common carp	http://www.hesiglobal.org/Committees/ProjectCommittees/Bioaccumulation/
Dieldrin	-1.75	Common carp	NITE. 2005. http://www.nite.go.jp/index-e.html
Dieldrin	-2.01	Common carp	NITE. 2005. http://www.nite.go.jp/index-e.html

[a]Values selected are the log $k_{M,N}$ from the Arnot et al (2008) database.

Notes

Chemical-specific metabolic transformation rate constants (K_m) for each chemical were obtained from Arnot et al (2008). The Kms were then normalized to water temperature and the mass of the organisms in each foodweb (see Tables 8a and 8b for species weights used in the foodwebs in this report) using the equation in Arnot et al (2008). If more than one chemical specific K_m was available in Arnot et al (2008), the geometric mean value was used.

$$K_{M,N} = K_{M,I} (W_N/W_i)^{-0.25} \exp[0.01(T_N-T_i)]$$

where:
$k_{M,i}$ = chemical-specific metabolic transformation rate from the literature
W_N = normalized mass of organism (10g)
W_i = study-specific mass of organisms
T_N = normalized water temperature (15 °C)
T_i = original study-specific temperature

References

Arnot, J.A., D. MacKay, T.F. Parkerton, M. Bonnell. 2008. A database of fish biotransformation rates for organic chemicals. Environmental Toxicology and Chemistry 27: 2263-2270.
Gobas, F.A.P. 1993. A Model for Predicting the Bioaccumulation Hydrophobic Organic Chemicals in Aquatic Food-webs: Application to Lake Ontario. Ecological Modelling, 69:1-17.

Table 10 - Summary of Normalized (to Water Temperature and Organism Weight) Metabolic Transformation Rate Constant (K_m) Inputs Used in the Gobas (1993) Model to Calculate Alternative Foodchain Multipliers

Foodweb	Foodweb Component	Species Weight (g)	Normalized K_m [a]					
			Benzo(a)pyrene		Fluoranthene		Dieldrin	
			8 °C	16 °C	8 °C	16 °C	8 °C	16 °C
Coldwater (Great Lakes)	Sculpin	5.4	0.6758	0.7321	1.1477	1.2433	0.0143	0.0155
	Alewife	32	0.4332	0.4692	0.5012	0.7969	0.0092	0.0100
	Smelt	16	0.5151	0.5580	0.5960	0.6456	0.0109	0.0118
	Salmonids	2,410	0.1470	0.1593	0.1701	0.1843	0.0031	0.0034
Warmwater	Panfish (sunfish)	200	0.2968	0.2740	0.3434	0.3170	0.0063	0.0058
	Largemouth bass	2,000	0.1669	0.1541	0.1931	0.1782	0.0035	0.0033
	Freshwater catfish	5,000	0.1327	0.1225	0.1536	0.1418	0.0028	0.0026

[a]See Table 9 for description of K_m equation and literature K_m values for each chemical. Values shown are the geometric means of the normalized (to water temperature and organism weight) K_ms for available chemical-specific K_ms from Arnot et al (2008)

Notes

K_m = metabolic transformation rate constant

C = Celsius

References

Arnot, J.A., D. MacKay, T.F. Parkerton, M. Bonnell. 2008. A database of fish biotransformation rates for organic chemicals. Environmental Toxicology and Chemistry 27: 2263-2270.

Gobas, F.A.P. 1993. A Model for Predicting the Bioaccumulation Hydrophobic Organic Chemicals in Aquatic Food-webs: Application to Lake Ontario. Ecological Modelling, 69:1-17.

Table 11a - USEPA and Gobas (1993) Foodweb Model Parameters (Based on Great Lakes Foodweb)

Species	Trophic Level	Lipid Content	Weight	Diet - Benthic Foodweb Model
Phytoplankton	1	0.5%	--	--
Zooplankton (i.e. *Mysis relicta*)	2	5%	--	--
Pontoporeia affinis	2	3%	--	--
Oligochaetes (*Tubifex tubifex*)	2	1%	--	--
Sculpin	3	8%	5.4 g	18% zooplankton, 82% *Pontoporeia*
Alewife	3	7%	32 g	60% zooplankton, 40% *Pontoporeia*
Smelt	3-4	4%	16 g	54% zooplankton, 21% *Pontoporeia* , 25% sculpin
Salmonids	4	11%	2,410 g	10% sculpin, 50% alewife, 40% smelt

Table 11b - Hypothetical Benthic and Pelagic Warmwater-based Foodweb Model Parameters

Species	Trophic Level	Lipid Content	Weight	Diet - Benthic Foodweb Model	Diet - Pelagic Foodweb Model
Phytoplankton	1	0.5%	--	--	--
Zooplankton	2	5%	100 mg	--	--
Crayfish	2	1%	6 g	--	--
Panfish (sunfish)	3	3%	200 g	20% zooplankton, 80% crayfish	80% zooplankton, 20% crayfish
Largemouth bass	4	4%	2,000 g	20% crayfish, 80% panfish	20% crayfish, 80% panfish
Freshwater catfish	4	8%	5,000 g	20% crayfish, 80% panfish	20% crayfish, 80% panfish

Reference

Gobas, F.A.P. 1993. A Model for Predicting the Bioaccumulation Hydrophobic Organic Chemicals in Aquatic Food-webs: Application to Lake Ontario. Ecological Modelling, 69:1-17.

Table 12 - National BAFs Resulting from Alternative Foodweb Model Scenarios

Foodweb	Metabolism (K_m)	Water Temperature (° C)	$\Pi_{SOCW/Kow}$	National BAFs (L/kg)				
				Benzo(a)pyrene	Fluoranthene	Dieldrin		
						TL 2	TL 3	TL 4
USEPA Default/Coldwater (Great Lakes)	0	8	23	3,900	1,500	14,000	215,000	404,000
Coldwater (Great Lakes)	Chemical-specific	8	23	900	1,500	14,000	120,000	126,000
Coldwater (Great Lakes)	Chemical-specific	8	10	500	1,500	14,000	58,000	63,000
Coldwater (Great Lakes)	Chemical-specific	8	2	300	1,500	14,000	19,000	25,000
Coldwater (Great Lakes)	Chemical-specific	16	23	800	1,500	14,000	160,000	221,000
Coldwater (Great Lakes)	Chemical-specific	16	10	600	1,500	14,000	76,000	109,000
Coldwater (Great Lakes)	Chemical-specific	16	2	300	1,500	14,000	24,000	40,000
Warmwater - benthic	Chemical-specific	8	23	800	1,400	14,000	151,000	150,000
Warmwater - benthic	Chemical-specific	8	10	600	1,400	14,000	72,000	71,000
Warmwater - benthic	Chemical-specific	8	2	300	1,400	14,000	24,000	17,000
Warmwater - benthic	Chemical-specific	16	23	1,000	1,400	14,000	199,000	236,000
Warmwater - benthic	Chemical-specific	16	10	700	1,400	14,000	94,000	111,000
Warmwater - benthic	Chemical-specific	16	2	400	1,400	14,000	30,000	25,000
Warmwater - pelagic	Chemical-specific	8	23	600	1,400	14,000	69,000	85,000
Warmwater - pelagic	Chemical-specific	8	10	500	1,400	14,000	50,000	54,000
Warmwater - pelagic	Chemical-specific	8	2	400	1,400	14,000	38,000	25,000
Warmwater - pelagic	Chemical-specific	16	23	700	1,400	14,000	90,000	128,000
Warmwater - pelagic	Chemical-specific	16	10	600	1,400	14,000	64,000	81,000
Warmwater - pelagic	Chemical-specific	16	2	500	1,400	14,000	48,000	39,000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

BAF = Bioaccumulation factor

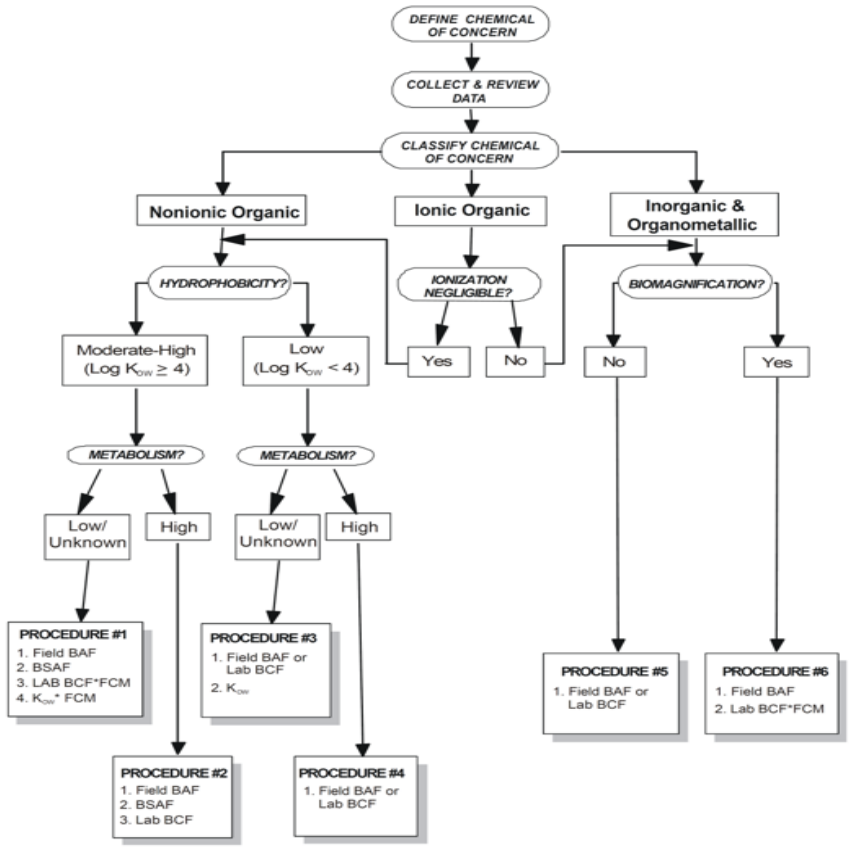
Table 13 - HHWQC Resulting from Alternative Foodweb Scenarios

Foodweb	Metabolism (K_m)	Water Temperature (° C)	$\Pi_{SOCW/Kow}$	HHWQC					
				Benzo(a)pyrene[a]		Fluoranthene[b]		Dieldrin[c]	
				Water and Organisms	Organisms Only	Water and Organisms	Organisms Only	Water and Organisms	Organisms Only
USEPA Default/Coldwater (Great Lakes)	0	8	23	1.24E-04	1.28E-04	18.1	19.4	1.24E-06	1.25E-06
Coldwater (Great Lakes)	Chemical-specific	8	23	4.94E-04	5.53E-04	18.1	19.4	2.80E-06	2.81E-06
Coldwater (Great Lakes)	Chemical-specific	8	10	8.18E-04	9.96E-04	18.1	19.4	5.38E-06	5.40E-06
Coldwater (Great Lakes)	Chemical-specific	8	2	1.22E-03	1.66E-03	18.1	19.4	1.25E-05	1.26E-05
Coldwater (Great Lakes)	Chemical-specific	16	23	5.48E-04	6.23E-04	18.1	19.4	1.91E-06	1.92E-06
Coldwater (Great Lakes)	Chemical-specific	16	10	7.02E-04	8.30E-04	18.1	19.4	3.79E-06	3.80E-06
Coldwater (Great Lakes)	Chemical-specific	16	2	1.22E-03	1.66E-03	18.1	19.4	9.63E-06	9.67E-06
Warmwater - benthic	Chemical-specific	8	23	5.48E-04	6.23E-04	19.3	20.8	2.30E-06	2.30E-06
Warmwater - benthic	Chemical-specific	8	10	7.02E-04	8.30E-04	19.3	20.8	4.59E-06	4.60E-06
Warmwater - benthic	Chemical-specific	8	2	1.22E-03	1.66E-03	19.3	20.8	1.24E-05	1.25E-05
Warmwater - benthic	Chemical-specific	16	23	4.49E-04	4.98E-04	19.3	20.8	1.65E-06	1.65E-06
Warmwater - benthic	Chemical-specific	16	10	6.16E-04	7.12E-04	19.3	20.8	3.37E-06	3.38E-06
Warmwater - benthic	Chemical-specific	16	2	9.78E-04	1.25E-03	19.3	20.8	1.01E-05	1.02E-05
Warmwater - pelagic	Chemical-specific	8	23	7.02E-04	8.30E-04	19.3	20.8	4.40E-06	4.41E-06
Warmwater - pelagic	Chemical-specific	8	10	8.18E-04	9.96E-04	19.3	20.8	6.14E-06	6.16E-06
Warmwater - pelagic	Chemical-specific	8	2	9.78E-04	1.25E-03	19.3	20.8	8.88E-06	8.92E-06
Warmwater - pelagic	Chemical-specific	16	23	6.16E-04	7.12E-04	19.3	20.8	3.26E-06	3.26E-06
Warmwater - pelagic	Chemical-specific	16	10	7.02E-04	8.30E-04	19.3	20.8	6.15E-06	6.17E-06
Warmwater - pelagic	Chemical-specific	16	2	8.18E-04	9.96E-04	19.3	20.8	6.94E-06	6.96E-06

[a]Carcinogenic HHWQCs shown for benzo(a)pyrene
[b]Non-carcinogenic HHWQCs shown for fluoranthene. Carcinogenic HHWQCs not available.
[c]Carcinogenic HHWQCs shown for dieldrin

Notes
K_{ow} = n-octanol-water partition coefficient
K_m = metabolic transformation rate constant
$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow
C = Celsius
HHWQC = human health water quality criteria

FIGURES



NOTES:

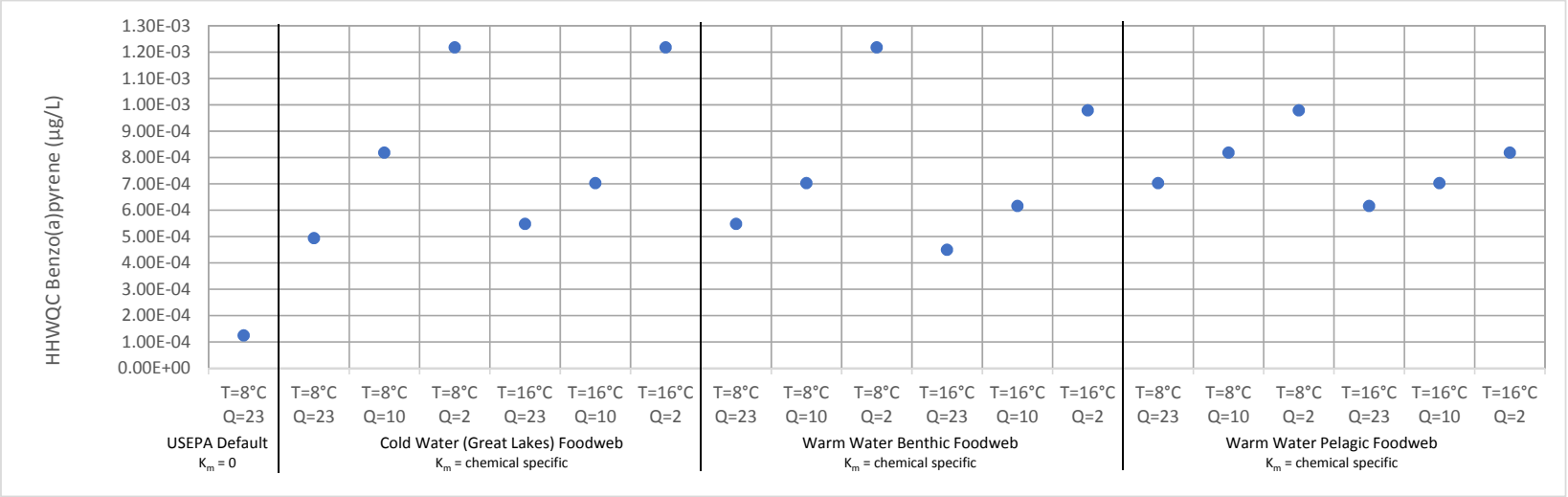
USEPA. 2003. Methodology for Deriving Ambient Water Quality Criteria for the Protection of Human Health (2000). Technical Support Document Volume 2: Development of National Bioaccumulation Factors. EPA-822-R-03-030

National Council for Air and Stream Improvement, (NCASI) Inc
FCM and BAF Refinement

Figure 1. Framework for selection of methods for deriving national BAFs from USEPA TSD Volume 2. (Figure 3-1 in USEPA 2003).

ARCADIS

Figure 1



NOTES:

T = Temperature
Q = $\Pi_{SOCW/Kow}$

K_{ow} = n-octanol-water partition coefficient
K_m = metabolic transformation rate constant
$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and K_{ow}
C = Celsius
HHWQC = human health water quality criteria

Carcinogenic HHWQCs shown for benzo(a)pyrene.

National Council for Air and Stream Improvement, (NCASI) Inc
FCM and BAF Refinement

Alternative Human Health Water Quality Criteria - Benzo(a)pyrene

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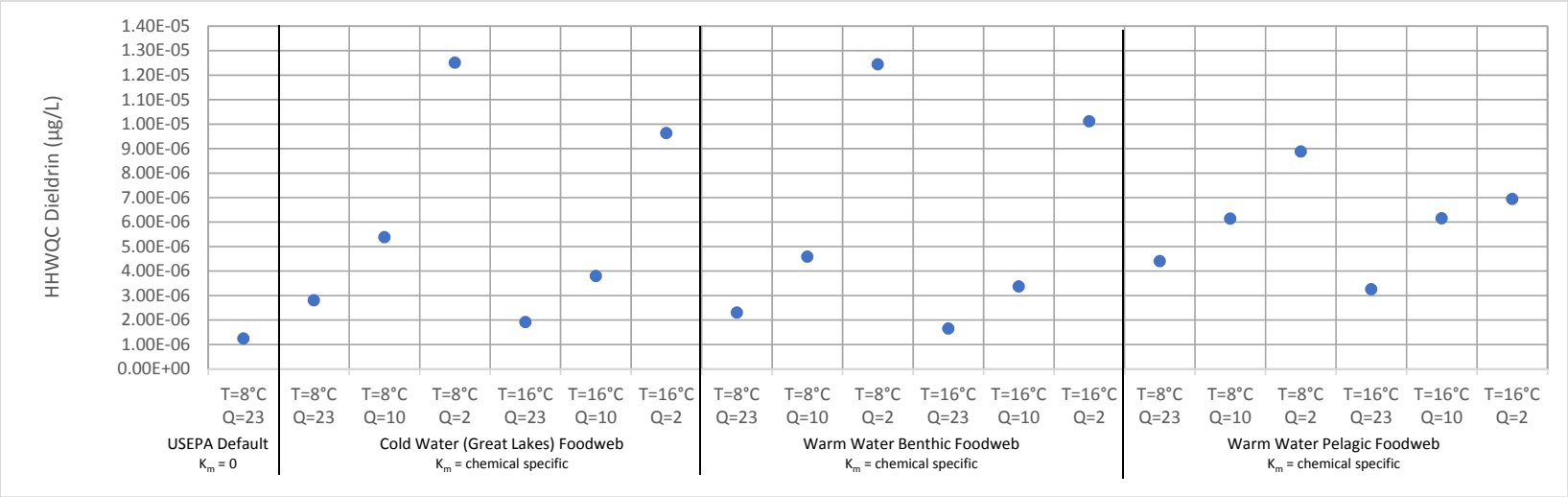
Figure 2



NOTES:

T = Temperature
Q = $\Pi_{SOCW/Kow}$

K_{ow} = n-octanol-water partition coefficient
K_m = metabolic transformation rate constant
$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and K_{ow}
C = Celsius
HHWQC = human health water quality criteria

Carcinogenic HHWQCs shown for dieldrin.

National Council for Air and Stream Improvement, (NCASI) Inc
FCM and BAF Refinement

Alternative Human Health Water Quality Criteria - Dieldrin

ARCADIS

Figure 3

APPENDIX A

Foodchain Multipliers at Specific K_{ow} for Alternative Sets of Assumptions

Table 1 - Summary of Normalized (to Water Temperature and Organism Weight) Metabolic Transformation Rate Constant (K_m) Inputs Used in the Gobas (1993) Model to Calculate Alternative Foodchain Multipliers

Foodweb	Foodweb Component	Species Weight (g)	Normalized K_m[1]					
			0.001		0.01		0.1	
			8 °C	16 °C	8 °C	16 °C	8 °C	16 °C
Coldwater (Great Lakes)	Sculpin	5.4	0.0011	0.0012	0.0109	0.0118	0.1088	0.1178
	Alewife	32	0.0007	0.0008	0.0070	0.0076	0.0697	0.0755
	Smelt	16	0.0008	0.0009	0.0083	0.0090	0.0829	0.0898
	Salmonids	2,410	0.0002	0.0003	0.0024	0.0026	0.0237	0.0256
Warmwater	Panfish (sunfish)	200	0.0004	0.0005	0.0044	0.0048	0.0441	0.0478
	Largemouth bass	2,000	0.0002	0.0003	0.0025	0.0027	0.0248	0.0269
	Freshwater catfish	5,000	0.0002	0.0002	0.0020	0.0021	0.0197	0.0214

[1]Kms were normalized to water temperature and the mass of the organisms in each foodweb using the equation in Arnot et al (2008):

$$K_{M,N} = K_{M,i} (W_N/W_i)^{-0.25} \exp[0.01(T_N - T_i)]$$

where:

$k_{M,i}$ = chemical-specific metabolic transformation rate from the literature

W_N = normalized mass of organism (10g)

W_i = study-specific mass of organisms

T_N = normalized water temperature (15 °C)

T_i = original study-specific temperature

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$SOCW/K_{ow}$ = ratio of sediment-water concentration quotient and K_{ow}

C = Celsius

FCM = Foodchain multiplier

TL = trophic level

References

Arnot, J.A., D. MacKay, T.F. Parkerton, M. Bonnell. 2008. A database of fish biotransformation rates for organic chemicals. Environmental Toxicology and Chemistry 27: 2263-2270.

Gobas, F.A.P. 1993. A Model for Predicting the Bioaccumulation Hydrophobic Organic Chemicals in Aquatic Food-webs: Application to Lake Ontario. Ecological Modelling, 69:1-17.

Table 2 - Foodchain Multipliers for USEPA Default Scenario, Great Lakes Foodweb Model
(Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.012	0.997
3.1	0.984	1.021	1.000
3.2	0.987	1.031	1.003
3.3	0.990	1.042	1.007
3.4	0.992	1.055	1.011
3.5	0.994	1.072	1.015
3.6	0.995	1.091	1.021
3.7	1.00	1.116	1.028
3.8	1.00	1.146	1.038
3.9	1.00	1.057	0.829
4.0	1.00	1.231	1.067
4.1	1.00	1.289	1.091
4.2	1.00	1.362	1.122
4.3	1.00	1.452	1.166
4.4	1.00	1.565	1.227
4.5	1.00	1.703	1.312
4.6	1.00	1.874	1.428
4.7	1.00	2.082	1.588
4.8	1.00	2.336	1.806
4.9	1.00	2.386	1.611
5.0	1.00	3.006	2.486
5.1	1.00	3.436	2.989
5.2	1.00	3.937	3.629
5.3	1.00	4.511	4.427
5.4	1.00	5.157	5.399
5.5	1.00	5.867	6.553
5.6	1.00	6.633	7.892
5.7	1.00	7.436	9.404
5.8	1.00	8.258	11.066
5.9	1.00	8.637	11.290
6.0	1.00	9.870	14.690
6.1	1.00	10.613	16.543
6.2	1.00	11.295	18.352
6.3	1.00	11.901	20.053
6.4	1.00	12.423	21.595
6.5	1.00	12.858	22.932
6.6	1.00	13.206	24.030
6.7	1.00	13.467	24.865
6.8	1.00	13.645	25.417
6.9	1.00	13.696	25.488
7.0	1.00	13.752	25.637
7.1	1.00	13.684	25.291
7.2	1.00	13.533	24.635
7.3	1.00	13.297	23.672
7.4	1.00	12.973	22.409
7.5	1.00	12.559	20.864
7.6	1.00	12.052	19.069
7.7	1.00	11.454	17.074
7.8	1.00	10.770	14.947
7.9	1.00	10.375	14.493
8.0	1.00	9.189	10.626
8.1	1.00	8.325	8.608
8.2	1.00	7.443	6.784
8.3	1.00	6.565	5.204
8.4	1.00	5.716	3.889
8.5	1.00	4.915	2.836
8.6	1.00	4.177	2.022
8.7	1.00	3.513	1.414
8.8	1.00	2.928	0.971
8.9	1.00	2.660	0.925
9.0	1.00	1.986	0.439
9.1	1.00	1.620	0.290
9.2	1.00	1.315	0.190
9.3	1.00	1.063	0.124
9.4	1.00	0.857	0.080
9.5	1.00	0.688	0.051
9.6	1.00	0.552	0.033
9.7	1.00	0.442	0.021
9.8	1.00	0.353	0.013
9.9	1.00	0.315	0.013

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 3 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.998	0.996
3.1	0.984	1.003	1.000
3.2	0.987	1.008	1.003
3.3	0.990	1.014	1.006
3.4	0.992	1.021	1.010
3.5	0.994	1.028	1.014
3.6	0.995	1.037	1.019
3.7	1.00	1.048	1.025
3.8	1.00	1.061	1.033
3.9	1.00	1.078	1.042
4.0	1.00	1.098	1.055
4.1	1.00	1.123	1.072
4.2	1.00	1.155	1.093
4.3	1.00	1.194	1.122
4.4	1.00	1.242	1.159
4.5	1.00	1.301	1.209
4.6	1.00	1.375	1.275
4.7	1.00	1.464	1.363
4.8	1.00	1.573	1.478
4.9	1.00	1.704	1.629
5.0	1.00	1.861	1.823
5.1	1.00	2.046	2.070
5.2	1.00	2.261	2.378
5.3	1.00	2.508	2.758
5.4	1.00	2.785	3.214
5.5	1.00	3.091	3.750
5.6	1.00	3.420	4.367
5.7	1.00	3.765	5.059
5.8	1.00	4.118	5.815
5.9	1.00	4.469	6.619
6.0	1.00	4.810	7.450
6.1	1.00	5.129	8.283
6.2	1.00	5.421	9.090
6.3	1.00	5.680	9.847
6.4	1.00	5.903	10.530
6.5	1.00	6.088	11.119
6.6	1.00	6.235	11.598
6.7	1.00	6.344	11.958
6.8	1.00	6.416	12.189
6.9	1.00	6.451	12.287
7.0	1.00	6.449	12.247
7.1	1.00	6.411	12.068
7.2	1.00	6.336	11.746
7.3	1.00	6.222	11.282
7.4	1.00	6.067	10.678
7.5	1.00	5.871	9.944
7.6	1.00	5.633	9.093
7.7	1.00	5.352	8.148
7.8	1.00	5.032	7.139
7.9	1.00	4.676	6.106
8.0	1.00	4.292	5.089
8.1	1.00	3.888	4.129
8.2	1.00	3.475	3.260
8.3	1.00	3.065	2.506
8.4	1.00	2.669	1.876
8.5	1.00	2.295	1.371
8.6	1.00	1.950	0.979
8.7	1.00	1.640	0.686
8.8	1.00	1.367	0.472
8.9	1.00	1.130	0.320
9.0	1.00	0.927	0.214
9.1	1.00	0.756	0.142
9.2	1.00	0.614	0.093
9.3	1.00	0.496	0.061
9.4	1.00	0.400	0.039
9.5	1.00	0.321	0.025
9.6	1.00	0.258	0.016
9.7	1.00	0.206	0.010
9.8	1.00	0.165	0.007
9.9	1.00	0.131	0.004

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 4 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.989	0.996
3.1	0.984	0.992	0.999
3.2	0.987	0.995	1.002
3.3	0.990	0.997	1.006
3.4	0.992	0.999	1.009
3.5	0.994	1.002	1.013
3.6	0.995	1.004	1.018
3.7	1.00	1.006	1.023
3.8	1.00	1.009	1.030
3.9	1.00	1.012	1.038
4.0	1.00	1.016	1.048
4.1	1.00	1.021	1.060
4.2	1.00	1.027	1.075
4.3	1.00	1.034	1.094
4.4	1.00	1.043	1.117
4.5	1.00	1.053	1.146
4.6	1.00	1.066	1.181
4.7	1.00	1.082	1.224
4.8	1.00	1.101	1.276
4.9	1.00	1.125	1.339
5.0	1.00	1.152	1.414
5.1	1.00	1.185	1.504
5.2	1.00	1.222	1.609
5.3	1.00	1.265	1.730
5.4	1.00	1.314	1.869
5.5	1.00	1.367	2.025
5.6	1.00	1.424	2.198
5.7	1.00	1.483	2.386
5.8	1.00	1.544	2.584
5.9	1.00	1.604	2.790
6.0	1.00	1.660	3.000
6.1	1.00	1.716	3.199
6.2	1.00	1.765	3.391
6.3	1.00	1.807	3.566
6.4	1.00	1.843	3.721
6.5	1.00	1.871	3.849
6.6	1.00	1.892	3.948
6.7	1.00	1.906	4.015
6.8	1.00	1.911	4.048
6.9	1.00	1.909	4.046
7.0	1.00	1.898	4.008
7.1	1.00	1.879	3.930
7.2	1.00	1.850	3.814
7.3	1.00	1.812	3.657
7.4	1.00	1.763	3.459
7.5	1.00	1.703	3.224
7.6	1.00	1.632	2.953
7.7	1.00	1.549	2.654
7.8	1.00	1.455	2.335
7.9	1.00	1.351	2.007
8.0	1.00	1.239	1.682
8.1	1.00	1.122	1.374
8.2	1.00	1.003	1.092
8.3	1.00	0.884	0.845
8.4	1.00	0.769	0.638
8.5	1.00	0.662	0.469
8.6	1.00	0.562	0.338
8.7	1.00	0.473	0.238
8.8	1.00	0.394	0.165
8.9	1.00	0.326	0.112
9.0	1.00	0.267	0.076
9.1	1.00	0.218	0.050
9.2	1.00	0.177	0.033
9.3	1.00	0.143	0.022
9.4	1.00	0.115	0.014
9.5	1.00	0.093	0.009
9.6	1.00	0.074	0.006
9.7	1.00	0.059	0.004
9.8	1.00	0.047	0.002
9.9	1.00	0.038	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 5 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.028	1.002
3.1	0.984	1.041	1.006
3.2	0.987	1.055	1.011
3.3	0.990	1.073	1.017
3.4	0.992	1.093	1.024
3.5	0.994	1.119	1.032
3.6	0.995	1.150	1.043
3.7	1.00	1.189	1.058
3.8	1.00	1.238	1.077
3.9	1.00	1.299	1.103
4.0	1.00	1.374	1.139
4.1	1.00	1.467	1.188
4.2	1.00	1.584	1.256
4.3	1.00	1.727	1.350
4.4	1.00	1.904	1.480
4.5	1.00	2.122	1.659
4.6	1.00	2.386	1.903
4.7	1.00	2.707	2.233
4.8	1.00	3.092	2.672
4.9	1.00	3.548	3.247
5.0	1.00	4.083	3.987
5.1	1.00	4.700	4.919
5.2	1.00	5.401	6.069
5.3	1.00	6.180	7.454
5.4	1.00	7.029	9.084
5.5	1.00	7.931	10.956
5.6	1.00	8.867	13.052
5.7	1.00	9.811	15.338
5.8	1.00	10.740	17.761
5.9	1.00	11.628	20.259
6.0	1.00	12.460	22.760
6.1	1.00	13.208	25.184
6.2	1.00	13.874	27.467
6.3	1.00	14.449	29.547
6.4	1.00	14.932	31.378
6.5	1.00	15.327	32.927
6.6	1.00	15.637	34.177
6.7	1.00	15.868	35.115
6.8	1.00	16.023	35.740
6.9	1.00	16.106	36.048
7.0	1.00	16.119	36.038
7.1	1.00	16.063	35.705
7.2	1.00	15.935	35.042
7.3	1.00	15.732	34.041
7.4	1.00	15.450	32.696
7.5	1.00	15.083	31.005
7.6	1.00	14.626	28.978
7.7	1.00	14.075	26.639
7.8	1.00	13.427	24.036
7.9	1.00	12.684	21.237
8.0	1.00	11.853	18.337
8.1	1.00	10.946	15.443
8.2	1.00	9.982	12.667
8.3	1.00	8.985	10.112
8.4	1.00	7.980	7.856
8.5	1.00	6.995	5.942
8.6	1.00	6.053	4.383
8.7	1.00	5.176	3.157
8.8	1.00	4.378	2.227
8.9	1.00	3.665	1.542
9.0	1.00	3.042	1.050
9.1	1.00	2.506	0.705
9.2	1.00	2.051	0.468
9.3	1.00	1.669	0.308
9.4	1.00	1.352	0.201
9.5	1.00	1.092	0.130
9.6	1.00	0.878	0.084
9.7	1.00	0.705	0.054
9.8	1.00	0.565	0.035
9.9	1.00	0.451	0.022

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 6 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.005	1.001
3.1	0.984	1.012	1.006
3.2	0.987	1.019	1.010
3.3	0.990	1.028	1.015
3.4	0.992	1.037	1.021
3.5	0.994	1.049	1.029
3.6	0.995	1.063	1.038
3.7	1.00	1.080	1.049
3.8	1.00	1.102	1.064
3.9	1.00	1.128	1.083
4.0	1.00	1.161	1.108
4.1	1.00	1.202	1.141
4.2	1.00	1.252	1.184
4.3	1.00	1.315	1.241
4.4	1.00	1.392	1.316
4.5	1.00	1.486	1.416
4.6	1.00	1.601	1.548
4.7	1.00	1.740	1.721
4.8	1.00	1.907	1.946
4.9	1.00	2.105	2.233
5.0	1.00	2.338	2.596
5.1	1.00	2.606	3.045
5.2	1.00	2.910	3.592
5.3	1.00	3.248	4.243
5.4	1.00	3.617	5.003
5.5	1.00	4.009	5.869
5.6	1.00	4.415	6.832
5.7	1.00	4.825	7.876
5.8	1.00	5.228	8.977
5.9	1.00	5.614	10.108
6.0	1.00	5.970	11.230
6.1	1.00	6.299	12.325
6.2	1.00	6.588	13.347
6.3	1.00	6.837	14.276
6.4	1.00	7.046	15.090
6.5	1.00	7.216	15.777
6.6	1.00	7.349	16.327
6.7	1.00	7.446	16.736
6.8	1.00	7.510	17.003
6.9	1.00	7.543	17.125
7.0	1.00	7.543	17.103
7.1	1.00	7.512	16.932
7.2	1.00	7.449	16.610
7.3	1.00	7.352	16.133
7.4	1.00	7.218	15.495
7.5	1.00	7.045	14.698
7.6	1.00	6.830	13.743
7.7	1.00	6.571	12.642
7.8	1.00	6.268	11.417
7.9	1.00	5.921	10.099
8.0	1.00	5.532	8.731
8.1	1.00	5.109	7.365
8.2	1.00	4.659	6.052
8.3	1.00	4.193	4.840
8.4	1.00	3.724	3.768
8.5	1.00	3.264	2.856
8.6	1.00	2.825	2.111
8.7	1.00	2.416	1.524
8.8	1.00	2.043	1.077
8.9	1.00	1.710	0.747
9.0	1.00	1.420	0.510
9.1	1.00	1.169	0.343
9.2	1.00	0.957	0.228
9.3	1.00	0.779	0.150
9.4	1.00	0.631	0.098
9.5	1.00	0.509	0.064
9.6	1.00	0.410	0.041
9.7	1.00	0.329	0.026
9.8	1.00	0.263	0.017
9.9	1.00	0.211	0.011

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 7 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.990	1.001
3.1	0.984	0.993	1.005
3.2	0.987	0.997	1.010
3.3	0.990	1.000	0.998
3.4	0.992	1.003	1.000
3.5	0.994	1.006	1.027
3.6	0.995	1.009	1.035
3.7	1.00	1.013	1.044
3.8	1.00	1.018	1.056
3.9	1.00	1.023	1.071
4.0	1.00	1.030	1.089
4.1	1.00	1.030	1.110
4.2	1.00	1.048	1.139
4.3	1.00	1.060	1.035
4.4	1.00	1.075	1.047
4.5	1.00	1.093	1.267
4.6	1.00	1.115	1.330
4.7	1.00	1.142	1.407
4.8	1.00	1.174	1.499
4.9	1.00	1.211	1.609
5.0	1.00	1.255	1.739
5.1	1.00	1.239	1.832
5.2	1.00	1.364	2.067
5.3	1.00	1.428	1.518
5.4	1.00	1.497	1.639
5.5	1.00	1.571	2.738
5.6	1.00	1.647	3.004
5.7	1.00	1.723	3.284
5.8	1.00	1.799	3.572
5.9	1.00	1.871	3.861
6.0	1.00	1.940	4.140
6.1	1.00	1.768	4.004
6.2	1.00	2.050	4.658
6.3	1.00	2.095	3.035
6.4	1.00	2.133	3.149
6.5	1.00	2.162	5.223
6.6	1.00	2.184	5.343
6.7	1.00	2.198	5.426
6.8	1.00	2.205	5.472
6.9	1.00	2.205	5.481
7.0	1.00	2.198	5.451
7.1	1.00	1.897	4.786
7.2	1.00	2.160	5.268
7.3	1.00	2.128	3.165
7.4	1.00	2.087	3.040
7.5	1.00	2.034	4.662
7.6	1.00	1.971	4.367
7.7	1.00	1.895	4.028
7.8	1.00	1.806	3.651
7.9	1.00	1.705	3.244
8.0	1.00	1.593	2.820
8.1	1.00	1.275	2.138
8.2	1.00	1.341	1.980
8.3	1.00	1.207	0.988
8.4	1.00	1.071	0.775
8.5	1.00	0.939	0.957
8.6	1.00	0.813	0.713
8.7	1.00	0.695	0.519
8.8	1.00	0.588	0.370
8.9	1.00	0.492	0.258
9.0	1.00	0.408	0.177
9.1	1.00	0.292	0.109
9.2	1.00	0.275	0.080
9.3	1.00	0.224	0.033
9.4	1.00	0.181	0.022
9.5	1.00	0.146	0.023
9.6	1.00	0.118	0.015
9.7	1.00	0.095	0.009
9.8	1.00	0.076	0.006
9.9	1.00	0.061	0.004

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 8 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi S_{OCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.012	0.996
3.1	0.984	1.021	0.999
3.2	0.987	1.031	1.002
3.3	0.990	1.042	1.006
3.4	0.992	1.055	1.009
3.5	0.994	1.071	1.014
3.6	0.995	1.091	1.019
3.7	1.00	1.115	1.026
3.8	1.00	1.145	1.035
3.9	1.00	1.056	0.827
4.0	1.00	1.229	1.063
4.1	1.00	1.287	1.085
4.2	1.00	1.359	1.115
4.3	1.00	1.449	1.157
4.4	1.00	1.560	1.215
4.5	1.00	1.696	1.296
4.6	1.00	1.864	1.407
4.7	1.00	2.070	1.560
4.8	1.00	2.318	1.767
4.9	1.00	2.366	1.576
5.0	1.00	2.972	2.409
5.1	1.00	3.390	2.881
5.2	1.00	3.873	3.477
5.3	1.00	4.424	4.214
5.4	1.00	5.039	5.103
5.5	1.00	5.710	6.151
5.6	1.00	6.428	7.354
5.7	1.00	7.174	8.697
5.8	1.00	7.931	10.157
5.9	1.00	8.274	10.339
6.0	1.00	9.390	13.277
6.1	1.00	10.055	14.843
6.2	1.00	10.656	16.346
6.3	1.00	11.184	17.736
6.4	1.00	11.633	18.971
6.5	1.00	12.000	20.015
6.6	1.00	12.285	20.843
6.7	1.00	12.490	21.435
6.8	1.00	12.616	21.779
6.9	1.00	12.641	21.802
7.0	1.00	12.634	21.688
7.1	1.00	12.526	21.244
7.2	1.00	12.339	20.533
7.3	1.00	12.069	19.559
7.4	1.00	11.715	18.334
7.5	1.00	11.274	16.882
7.6	1.00	10.748	15.241
7.7	1.00	10.140	13.461
7.8	1.00	9.458	11.611
7.9	1.00	9.070	11.238
8.0	1.00	7.926	7.993
8.1	1.00	7.113	6.368
8.2	1.00	6.298	4.938
8.3	1.00	5.503	3.729
8.4	1.00	4.748	2.746
8.5	1.00	4.049	1.976
8.6	1.00	3.415	1.393
8.7	1.00	2.853	0.964
8.8	1.00	2.363	0.656
8.9	1.00	2.142	0.626
9.0	1.00	1.588	0.293
9.1	1.00	1.291	0.192
9.2	1.00	1.045	0.126
9.3	1.00	0.843	0.081
9.4	1.00	0.677	0.053
9.5	1.00	0.543	0.034
9.6	1.00	0.435	0.022
9.7	1.00	0.348	0.014
9.8	1.00	0.278	0.009
9.9	1.00	0.248	0.008

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 9 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.997	0.996
3.1	0.984	1.003	0.999
3.2	0.987	1.008	1.002
3.3	0.990	1.014	1.005
3.4	0.992	1.020	1.009
3.5	0.994	1.028	1.012
3.6	0.995	1.037	1.017
3.7	1.00	1.047	1.023
3.8	1.00	1.060	1.030
3.9	1.00	1.077	1.039
4.0	1.00	1.097	1.051
4.1	1.00	1.121	1.066
4.2	1.00	1.152	1.086
4.3	1.00	1.191	1.113
4.4	1.00	1.238	1.148
4.5	1.00	1.296	1.195
4.6	1.00	1.368	1.257
4.7	1.00	1.455	1.339
4.8	1.00	1.561	1.447
4.9	1.00	1.689	1.587
5.0	1.00	1.840	1.764
5.1	1.00	2.018	1.997
5.2	1.00	2.225	2.281
5.3	1.00	2.459	2.628
5.4	1.00	2.722	3.042
5.5	1.00	3.008	3.525
5.6	1.00	3.314	4.075
5.7	1.00	3.632	4.685
5.8	1.00	3.955	5.344
5.9	1.00	4.272	6.037
6.0	1.00	4.576	6.375
6.1	1.00	4.859	7.441
6.2	1.00	5.115	8.108
6.3	1.00	5.339	8.722
6.4	1.00	5.528	9.265
6.5	1.00	5.682	9.720
6.6	1.00	5.800	10.077
6.7	1.00	5.884	10.327
6.8	1.00	5.932	10.464
6.9	1.00	5.945	10.483
7.0	1.00	5.925	9.115
7.1	1.00	5.869	10.158
7.2	1.00	5.777	9.811
7.3	1.00	5.647	9.342
7.4	1.00	5.479	8.757
7.5	1.00	5.271	8.066
7.6	1.00	5.023	7.286
7.7	1.00	4.738	6.441
7.8	1.00	4.418	5.561
7.9	1.00	4.070	4.682
8.0	1.00	3.702	3.404
8.1	1.00	3.322	3.064
8.2	1.00	2.941	2.380
8.3	1.00	2.570	1.800
8.4	1.00	2.217	1.328
8.5	1.00	1.890	0.958
8.6	1.00	1.595	0.676
8.7	1.00	1.332	0.469
8.8	1.00	1.103	0.320
8.9	1.00	0.907	0.215
9.0	1.00	0.741	0.139
9.1	1.00	0.603	0.094
9.2	1.00	0.488	0.061
9.3	1.00	0.393	0.040
9.4	1.00	0.316	0.026
9.5	1.00	0.254	0.017
9.6	1.00	0.203	0.011
9.7	1.00	0.162	0.007
9.8	1.00	0.130	0.004
9.9	1.00	0.103	0.003

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 10 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.988	0.996
3.1	0.984	0.992	0.999
3.2	0.987	0.994	1.002
3.3	0.990	0.997	1.005
3.4	0.992	0.999	1.008
3.5	0.994	1.001	1.012
3.6	0.995	1.003	1.016
3.7	1.00	1.006	1.021
3.8	1.00	1.008	1.027
3.9	1.00	1.011	1.034
4.0	1.00	1.015	1.043
4.1	1.00	1.019	1.054
4.2	1.00	1.025	1.068
4.3	1.00	1.031	1.085
4.4	1.00	1.039	1.107
4.5	1.00	1.049	1.133
4.6	1.00	1.061	1.164
4.7	1.00	1.076	1.203
4.8	1.00	1.093	1.250
4.9	1.00	1.114	1.306
5.0	1.00	1.139	1.373
5.1	1.00	1.169	1.453
5.2	1.00	1.202	1.545
5.3	1.00	1.241	1.652
5.4	1.00	1.284	1.773
5.5	1.00	1.330	1.908
5.6	1.00	1.380	2.057
5.7	1.00	1.431	2.216
5.8	1.00	1.483	2.383
5.9	1.00	1.533	2.553
6.0	1.00	1.581	2.723
6.1	1.00	1.625	2.886
6.2	1.00	1.665	3.039
6.3	1.00	1.698	3.175
6.4	1.00	1.726	3.292
6.5	1.00	1.746	3.385
6.6	1.00	1.760	3.452
6.7	1.00	1.767	3.491
6.8	1.00	1.767	3.500
6.9	1.00	1.759	3.478
7.0	1.00	1.744	3.424
7.1	1.00	1.720	3.336
7.2	1.00	1.687	3.213
7.3	1.00	1.645	3.055
7.4	1.00	1.592	2.864
7.5	1.00	1.529	2.641
7.6	1.00	1.455	2.391
7.7	1.00	1.371	2.120
7.8	1.00	1.277	1.838
7.9	1.00	1.176	1.556
8.0	1.00	1.069	1.283
8.1	1.00	0.959	1.031
8.2	1.00	0.848	0.806
8.3	1.00	0.741	0.614
8.4	1.00	0.639	0.456
8.5	1.00	0.545	0.331
8.6	1.00	0.460	0.235
8.7	1.00	0.384	0.164
8.8	1.00	0.318	0.112
8.9	1.00	0.261	0.076
9.0	1.00	0.214	0.051
9.1	1.00	0.174	0.034
9.2	1.00	0.141	0.022
9.3	1.00	0.113	0.014
9.4	1.00	0.091	0.009
9.5	1.00	0.073	0.006
9.6	1.00	0.059	0.004
9.7	1.00	0.047	0.002
9.8	1.00	0.037	0.002
9.9	1.00	0.030	0.001

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 11 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.028	1.001
3.1	0.984	1.041	1.006
3.2	0.987	1.055	1.010
3.3	0.990	1.072	1.016
3.4	0.992	1.093	1.023
3.5	0.994	1.118	1.031
3.6	0.995	1.150	1.041
3.7	1.00	1.189	1.055
3.8	1.00	1.237	1.074
3.9	1.00	1.297	1.099
4.0	1.00	1.372	1.134
4.1	1.00	1.465	1.182
4.2	1.00	1.580	1.248
4.3	1.00	1.723	1.339
4.4	1.00	1.898	1.465
4.5	1.00	2.113	1.638
4.6	1.00	2.374	1.874
4.7	1.00	2.690	2.191
4.8	1.00	3.068	2.613
4.9	1.00	3.515	3.163
5.0	1.00	4.036	3.849
5.1	1.00	4.636	4.748
5.2	1.00	5.313	5.829
5.3	1.00	6.063	7.122
5.4	1.00	6.874	8.632
5.5	1.00	7.730	10.353
5.6	1.00	8.612	12.262
5.7	1.00	9.496	14.325
5.8	1.00	10.358	16.492
5.9	1.00	11.177	18.702
6.0	1.00	11.934	19.428
6.1	1.00	12.616	22.990
6.2	1.00	13.215	24.942
6.3	1.00	13.727	26.696
6.4	1.00	14.153	28.216
6.5	1.00	14.494	29.474
6.6	1.00	14.755	30.456
6.7	1.00	14.941	31.155
6.8	1.00	15.053	31.564
6.9	1.00	15.096	31.683
7.0	1.00	15.069	27.351
7.1	1.00	14.972	31.031
7.2	1.00	14.802	30.249
7.3	1.00	14.555	29.156
7.4	1.00	14.228	27.749
7.5	1.00	13.815	26.037
7.6	1.00	13.311	24.038
7.7	1.00	12.716	21.791
7.8	1.00	12.030	19.354
7.9	1.00	11.260	16.806
8.0	1.00	10.416	12.192
8.1	1.00	9.515	11.757
8.2	1.00	8.579	9.449
8.3	1.00	7.633	7.391
8.4	1.00	6.702	5.629
8.5	1.00	5.809	4.179
8.6	1.00	4.975	3.029
8.7	1.00	4.213	2.149
8.8	1.00	3.532	1.495
8.9	1.00	2.935	1.023
9.0	1.00	2.419	0.655
9.1	1.00	1.982	0.460
9.2	1.00	1.614	0.303
9.3	1.00	1.308	0.198
9.4	1.00	1.056	0.129
9.5	1.00	0.850	0.083
9.6	1.00	0.683	0.053
9.7	1.00	0.547	0.034
9.8	1.00	0.437	0.022
9.9	1.00	0.349	0.014

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 12 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.005	1.001
3.1	0.984	1.011	1.005
3.2	0.987	1.019	1.009
3.3	0.990	1.027	1.014
3.4	0.992	1.037	1.020
3.5	0.994	1.049	1.027
3.6	0.995	1.063	1.036
3.7	1.00	1.080	1.047
3.8	1.00	1.101	1.061
3.9	1.00	1.127	1.079
4.0	1.00	1.159	1.103
4.1	1.00	1.200	1.134
4.2	1.00	1.250	1.176
4.3	1.00	1.311	1.230
4.4	1.00	1.387	1.303
4.5	1.00	1.480	1.399
4.6	1.00	1.593	1.525
4.7	1.00	1.729	1.691
4.8	1.00	1.892	1.904
4.9	1.00	2.085	2.177
5.0	1.00	2.311	2.509
5.1	1.00	2.570	2.942
5.2	1.00	2.863	3.452
5.3	1.00	3.187	4.058
5.4	1.00	3.537	4.758
5.5	1.00	3.907	5.550
5.6	1.00	4.288	6.424
5.7	1.00	4.670	7.362
5.8	1.00	5.043	8.343
5.9	1.00	5.396	9.340
6.0	1.00	5.723	9.656
6.1	1.00	6.017	11.263
6.2	1.00	6.275	12.134
6.3	1.00	6.496	12.914
6.4	1.00	6.678	13.587
6.5	1.00	6.824	14.142
6.6	1.00	6.934	14.571
6.7	1.00	7.011	14.871
6.8	1.00	7.056	15.040
6.9	1.00	7.069	15.076
7.0	1.00	7.052	13.128
7.1	1.00	7.002	14.742
7.2	1.00	6.919	14.365
7.3	1.00	6.802	13.844
7.4	1.00	6.647	13.178
7.5	1.00	6.452	12.369
7.6	1.00	6.216	11.426
7.7	1.00	5.937	10.366
7.8	1.00	5.616	9.217
7.9	1.00	5.256	8.013
8.0	1.00	4.862	5.890
8.1	1.00	4.441	5.624
8.2	1.00	4.004	4.528
8.3	1.00	3.562	3.549
8.4	1.00	3.128	2.708
8.5	1.00	2.711	2.015
8.6	1.00	2.322	1.463
8.7	1.00	1.966	1.040
8.8	1.00	1.648	0.725
8.9	1.00	1.369	0.497
9.0	1.00	1.129	0.320
9.1	1.00	0.925	0.224
9.2	1.00	0.753	0.148
9.3	1.00	0.610	0.097
9.4	1.00	0.493	0.063
9.5	1.00	0.397	0.041
9.6	1.00	0.319	0.026
9.7	1.00	0.255	0.017
9.8	1.00	0.204	0.011
9.9	1.00	0.163	0.007

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 13 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.990	1.000
3.1	0.984	0.993	1.004
3.2	0.987	0.997	1.009
3.3	0.990	1.000	0.997
3.4	0.992	1.003	0.999
3.5	0.994	1.006	1.025
3.6	0.995	1.009	1.033
3.7	1.00	1.013	1.042
3.8	1.00	1.017	1.053
3.9	1.00	1.022	1.067
4.0	1.00	1.028	1.084
4.1	1.00	1.028	1.104
4.2	1.00	1.046	1.132
4.3	1.00	1.057	1.027
4.4	1.00	1.071	1.037
4.5	1.00	1.088	1.252
4.6	1.00	1.109	1.311
4.7	1.00	1.134	1.382
4.8	1.00	1.164	1.468
4.9	1.00	1.200	1.570
5.0	1.00	1.241	1.690
5.1	1.00	1.222	1.773
5.2	1.00	1.342	1.990
5.3	1.00	1.400	1.456
5.4	1.00	1.464	1.564
5.5	1.00	1.531	2.595
5.6	1.00	1.599	2.831
5.7	1.00	1.668	3.078
5.8	1.00	1.735	3.329
5.9	1.00	1.798	3.579
6.0	1.00	1.856	3.820
6.1	1.00	1.689	3.676
6.2	1.00	1.953	4.253
6.3	1.00	1.991	2.759
6.4	1.00	2.021	2.850
6.5	1.00	2.044	4.706
6.6	1.00	2.061	4.795
6.7	1.00	2.070	4.850
6.8	1.00	2.072	4.871
6.9	1.00	2.067	4.856
7.0	1.00	2.055	4.806
7.1	1.00	1.769	4.202
7.2	1.00	2.007	4.590
7.3	1.00	1.969	2.738
7.4	1.00	1.921	2.607
7.5	1.00	1.863	3.958
7.6	1.00	1.793	3.665
7.7	1.00	1.712	3.336
7.8	1.00	1.618	2.978
7.9	1.00	1.514	2.602
8.0	1.00	1.400	2.221
8.1	1.00	1.109	1.655
8.2	1.00	1.152	1.500
8.3	1.00	1.025	0.733
8.4	1.00	0.900	0.564
8.5	1.00	0.780	0.683
8.6	1.00	0.668	0.500
8.7	1.00	0.565	0.358
8.8	1.00	0.474	0.251
8.9	1.00	0.394	0.173
9.0	1.00	0.325	0.118
9.1	1.00	0.231	0.071
9.2	1.00	0.217	0.052
9.3	1.00	0.176	0.021
9.4	1.00	0.142	0.014
9.5	1.00	0.114	0.015
9.6	1.00	0.092	0.009
9.7	1.00	0.073	0.006
9.8	1.00	0.059	0.004
9.9	1.00	0.047	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 14 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.011	0.992
3.1	0.984	1.019	0.994
3.2	0.987	1.029	0.996
3.3	0.990	1.039	0.998
3.4	0.992	1.052	1.000
3.5	0.994	1.067	1.002
3.6	0.995	1.086	1.004
3.7	1.00	1.108	1.007
3.8	1.00	1.137	1.011
3.9	1.00	1.047	0.808
4.0	1.00	1.215	1.026
4.1	1.00	1.269	1.038
4.2	1.00	1.335	1.055
4.3	1.00	1.416	1.081
4.4	1.00	1.517	1.118
4.5	1.00	1.639	1.169
4.6	1.00	1.786	1.241
4.7	1.00	1.963	1.340
4.8	1.00	2.173	1.471
4.9	1.00	2.202	1.306
5.0	1.00	2.701	1.863
5.1	1.00	3.022	2.135
5.2	1.00	3.379	2.463
5.3	1.00	3.766	2.847
5.4	1.00	4.177	3.284
5.5	1.00	4.602	3.766
5.6	1.00	5.030	4.282
5.7	1.00	5.447	4.816
5.8	1.00	5.845	5.353
5.9	1.00	6.003	5.372
6.0	1.00	6.540	6.365
6.1	1.00	6.825	6.807
6.2	1.00	7.064	7.189
6.3	1.00	7.256	7.501
6.4	1.00	7.401	7.737
6.5	1.00	7.498	7.890
6.6	1.00	7.550	7.958
6.7	1.00	7.557	7.938
6.8	1.00	7.517	7.827
6.9	1.00	7.470	7.784
7.0	1.00	7.297	7.332
7.1	1.00	7.113	6.950
7.2	1.00	6.879	6.482
7.3	1.00	6.593	5.939
7.4	1.00	6.257	5.334
7.5	1.00	5.874	4.687
7.6	1.00	5.449	4.022
7.7	1.00	4.992	3.365
7.8	1.00	4.514	2.741
7.9	1.00	4.259	2.651
8.0	1.00	3.544	1.679
8.1	1.00	3.079	1.264
8.2	1.00	2.643	0.928
8.3	1.00	2.242	0.666
8.4	1.00	1.883	0.469
8.5	1.00	1.567	0.324
8.6	1.00	1.294	0.220
8.7	1.00	1.061	0.148
8.8	1.00	0.865	0.098
8.9	1.00	0.778	0.094
9.0	1.00	0.567	0.042
9.1	1.00	0.456	0.027
9.2	1.00	0.367	0.018
9.3	1.00	0.294	0.011
9.4	1.00	0.235	0.007
9.5	1.00	0.188	0.005
9.6	1.00	0.150	0.003
9.7	1.00	0.119	0.002
9.8	1.00	0.095	0.001
9.9	1.00	0.085	0.001

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 15 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.996	0.992
3.1	0.984	1.001	0.994
3.2	0.987	1.006	0.996
3.3	0.990	1.011	0.997
3.4	0.992	1.017	0.999
3.5	0.994	1.024	1.000
3.6	0.995	1.032	1.002
3.7	1.00	1.041	1.004
3.8	1.00	1.053	1.006
3.9	1.00	1.067	1.010
4.0	1.00	1.084	1.014
4.1	1.00	1.105	1.020
4.2	1.00	1.132	1.028
4.3	1.00	1.164	1.040
4.4	1.00	1.204	1.057
4.5	1.00	1.252	1.080
4.6	1.00	1.310	1.112
4.7	1.00	1.380	1.155
4.8	1.00	1.463	1.211
4.9	1.00	1.560	1.285
5.0	1.00	1.673	1.379
5.1	1.00	1.799	1.494
5.2	1.00	1.941	1.633
5.3	1.00	2.094	1.795
5.4	1.00	2.256	1.979
5.5	1.00	2.424	2.181
5.6	1.00	2.593	2.397
5.7	1.00	2.758	2.620
5.8	1.00	2.915	2.844
5.9	1.00	3.059	3.061
6.0	1.00	3.187	3.263
6.1	1.00	3.298	3.445
6.2	1.00	3.391	3.601
6.3	1.00	3.464	3.725
6.4	1.00	3.517	3.816
6.5	1.00	3.551	3.871
6.6	1.00	3.565	3.888
6.7	1.00	3.560	3.865
6.8	1.00	3.535	3.802
6.9	1.00	3.489	3.697
7.0	1.00	3.422	3.550
7.1	1.00	3.333	3.362
7.2	1.00	3.220	3.134
7.3	1.00	3.085	2.871
7.4	1.00	2.926	2.579
7.5	1.00	2.746	2.267
7.6	1.00	2.547	1.946
7.7	1.00	2.333	1.630
7.8	1.00	2.109	1.329
7.9	1.00	1.881	1.055
8.0	1.00	1.655	0.816
8.1	1.00	1.438	0.615
8.2	1.00	1.234	0.452
8.3	1.00	1.047	0.325
8.4	1.00	0.879	0.229
8.5	1.00	0.732	0.158
8.6	1.00	0.604	0.108
8.7	1.00	0.495	0.072
8.8	1.00	0.404	0.048
8.9	1.00	0.327	0.032
9.0	1.00	0.265	0.021
9.1	1.00	0.213	0.013
9.2	1.00	0.171	0.009
9.3	1.00	0.137	0.006
9.4	1.00	0.110	0.004
9.5	1.00	0.088	0.002
9.6	1.00	0.070	0.001
9.7	1.00	0.056	0.001
9.8	1.00	0.044	0.001
9.9	1.00	0.035	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 16 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.987	0.992
3.1	0.984	0.990	0.994
3.2	0.987	0.992	0.995
3.3	0.990	0.994	0.997
3.4	0.992	0.996	0.998
3.5	0.994	0.997	0.999
3.6	0.995	0.999	1.001
3.7	1.00	1.000	1.002
3.8	1.00	1.001	1.003
3.9	1.00	1.002	1.005
4.0	1.00	1.003	1.007
4.1	1.00	1.005	1.009
4.2	1.00	1.006	1.012
4.3	1.00	1.008	1.015
4.4	1.00	1.010	1.019
4.5	1.00	1.013	1.025
4.6	1.00	1.016	1.032
4.7	1.00	1.020	1.041
4.8	1.00	1.024	1.051
4.9	1.00	1.030	1.065
5.0	1.00	1.035	1.081
5.1	1.00	1.042	1.100
5.2	1.00	1.049	1.122
5.3	1.00	1.056	1.148
5.4	1.00	1.064	1.176
5.5	1.00	1.072	1.206
5.6	1.00	1.080	1.237
5.7	1.00	1.086	1.269
5.8	1.00	1.093	1.300
5.9	1.00	1.098	1.329
6.0	1.00	1.101	1.355
6.1	1.00	1.103	1.376
6.2	1.00	1.104	1.392
6.3	1.00	1.102	1.402
6.4	1.00	1.098	1.404
6.5	1.00	1.091	1.398
6.6	1.00	1.082	1.383
6.7	1.00	1.069	1.359
6.8	1.00	1.053	1.325
6.9	1.00	1.032	1.279
7.0	1.00	1.007	1.222
7.1	1.00	0.977	1.153
7.2	1.00	0.940	1.073
7.3	1.00	0.898	0.982
7.4	1.00	0.850	0.883
7.5	1.00	0.797	0.777
7.6	1.00	0.738	0.669
7.7	1.00	0.675	0.562
7.8	1.00	0.610	0.460
7.9	1.00	0.543	0.367
8.0	1.00	0.478	0.285
8.1	1.00	0.415	0.215
8.2	1.00	0.356	0.159
8.3	1.00	0.302	0.115
8.4	1.00	0.254	0.081
8.5	1.00	0.211	0.056
8.6	1.00	0.174	0.039
8.7	1.00	0.143	0.026
8.8	1.00	0.116	0.017
8.9	1.00	0.094	0.011
9.0	1.00	0.076	0.008
9.1	1.00	0.061	0.005
9.2	1.00	0.049	0.003
9.3	1.00	0.040	0.002
9.4	1.00	0.032	0.001
9.5	1.00	0.025	0.001
9.6	1.00	0.020	0.001
9.7	1.00	0.016	0.000
9.8	1.00	0.013	0.000
9.9	1.00	0.010	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 17 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.027	0.997
3.1	0.984	1.039	1.000
3.2	0.987	1.053	1.003
3.3	0.990	1.069	1.007
3.4	0.992	1.089	1.012
3.5	0.994	1.114	1.017
3.6	0.995	1.144	1.025
3.7	1.00	1.181	1.034
3.8	1.00	1.227	1.048
3.9	1.00	1.284	1.066
4.0	1.00	1.355	1.091
4.1	1.00	1.442	1.126
4.2	1.00	1.550	1.176
4.3	1.00	1.682	1.245
4.4	1.00	1.842	1.340
4.5	1.00	2.036	1.469
4.6	1.00	2.269	1.643
4.7	1.00	2.545	1.872
4.8	1.00	2.868	2.167
4.9	1.00	3.240	2.541
5.0	1.00	3.661	3.001
5.1	1.00	4.129	3.553
5.2	1.00	4.637	4.198
5.3	1.00	5.176	4.932
5.4	1.00	5.733	5.742
5.5	1.00	6.293	6.613
5.6	1.00	6.841	7.521
5.7	1.00	7.364	8.440
5.8	1.00	7.847	9.342
5.9	1.00	8.284	10.199
6.0	1.00	8.666	10.988
6.1	1.00	8.992	11.688
6.2	1.00	9.260	12.284
6.3	1.00	9.473	12.765
6.4	1.00	9.630	13.125
6.5	1.00	9.736	13.359
6.6	1.00	9.790	13.466
6.7	1.00	9.794	13.443
6.8	1.00	9.748	13.288
6.9	1.00	9.651	12.998
7.0	1.00	9.501	12.571
7.1	1.00	9.294	12.006
7.2	1.00	9.029	11.307
7.3	1.00	8.703	10.481
7.4	1.00	8.315	9.543
7.5	1.00	7.867	8.517
7.6	1.00	7.362	7.436
7.7	1.00	6.809	6.339
7.8	1.00	6.218	5.268
7.9	1.00	5.604	4.263
8.0	1.00	4.984	3.359
8.1	1.00	4.374	2.578
8.2	1.00	3.790	1.928
8.3	1.00	3.244	1.408
8.4	1.00	2.746	1.006
8.5	1.00	2.302	0.704
8.6	1.00	1.912	0.485
8.7	1.00	1.576	0.329
8.8	1.00	1.290	0.220
8.9	1.00	1.051	0.146
9.0	1.00	0.852	0.096
9.1	1.00	0.687	0.062
9.2	1.00	0.553	0.040
9.3	1.00	0.444	0.026
9.4	1.00	0.356	0.017
9.5	1.00	0.285	0.011
9.6	1.00	0.227	0.007
9.7	1.00	0.181	0.004
9.8	1.00	0.145	0.003
9.9	1.00	0.115	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 18 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.003	0.996
3.1	0.984	1.010	0.999
3.2	0.987	1.017	1.003
3.3	0.990	1.025	1.006
3.4	0.992	1.034	1.010
3.5	0.994	1.044	1.014
3.6	0.995	1.057	1.019
3.7	1.00	1.073	1.026
3.8	1.00	1.092	1.035
3.9	1.00	1.116	1.046
4.0	1.00	1.145	1.062
4.1	1.00	1.181	1.082
4.2	1.00	1.226	1.109
4.3	1.00	1.280	1.146
4.4	1.00	1.346	1.194
4.5	1.00	1.426	1.258
4.6	1.00	1.522	1.342
4.7	1.00	1.636	1.451
4.8	1.00	1.769	1.589
4.9	1.00	1.922	1.760
5.0	1.00	2.096	1.969
5.1	1.00	2.289	2.217
5.2	1.00	2.498	2.505
5.3	1.00	2.720	2.831
5.4	1.00	2.950	3.188
5.5	1.00	3.181	3.571
5.6	1.00	3.406	3.968
5.7	1.00	3.621	4.368
5.8	1.00	3.820	4.760
5.9	1.00	3.999	5.131
6.0	1.00	4.156	5.471
6.1	1.00	4.289	5.771
6.2	1.00	4.397	6.025
6.3	1.00	4.482	6.227
6.4	1.00	4.544	6.376
6.5	1.00	4.583	6.468
6.6	1.00	4.601	6.503
6.7	1.00	4.596	6.478
6.8	1.00	4.569	6.394
6.9	1.00	4.520	6.248
7.0	1.00	4.446	6.038
7.1	1.00	4.347	5.765
7.2	1.00	4.221	5.428
7.3	1.00	4.067	5.033
7.4	1.00	3.885	4.584
7.5	1.00	3.674	4.094
7.6	1.00	3.438	3.578
7.7	1.00	3.179	3.053
7.8	1.00	2.903	2.540
7.9	1.00	2.616	2.059
8.0	1.00	2.326	1.624
8.1	1.00	2.042	1.248
8.2	1.00	1.769	0.935
8.3	1.00	1.514	0.684
8.4	1.00	1.282	0.489
8.5	1.00	1.074	0.343
8.6	1.00	0.892	0.236
8.7	1.00	0.735	0.160
8.8	1.00	0.602	0.107
8.9	1.00	0.490	0.071
9.0	1.00	0.397	0.047
9.1	1.00	0.321	0.030
9.2	1.00	0.258	0.020
9.3	1.00	0.207	0.013
9.4	1.00	0.166	0.008
9.5	1.00	0.133	0.005
9.6	1.00	0.106	0.003
9.7	1.00	0.085	0.002
9.8	1.00	0.067	0.001
9.9	1.00	0.054	0.001

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 19 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.989	0.996
3.1	0.984	0.991	0.999
3.2	0.987	0.994	1.002
3.3	0.990	0.997	0.989
3.4	0.992	0.999	0.988
3.5	0.994	1.001	1.012
3.6	0.995	1.004	1.016
3.7	1.00	1.006	1.021
3.8	1.00	1.009	1.027
3.9	1.00	1.012	1.035
4.0	1.00	1.016	1.044
4.1	1.00	1.012	1.053
4.2	1.00	1.025	1.068
4.3	1.00	1.032	0.959
4.4	1.00	1.040	0.954
4.5	1.00	1.049	1.129
4.6	1.00	1.060	1.158
4.7	1.00	1.073	1.192
4.8	1.00	1.088	1.233
4.9	1.00	1.106	1.280
5.0	1.00	1.126	1.334
5.1	1.00	1.088	1.353
5.2	1.00	1.171	1.464
5.3	1.00	1.196	1.042
5.4	1.00	1.221	1.076
5.5	1.00	1.246	1.698
5.6	1.00	1.271	1.781
5.7	1.00	1.293	1.862
5.8	1.00	1.314	1.940
5.9	1.00	1.333	2.012
6.0	1.00	1.348	2.076
6.1	1.00	1.204	1.943
6.2	1.00	1.369	2.173
6.3	1.00	1.374	1.376
6.4	1.00	1.375	1.385
6.5	1.00	1.373	2.227
6.6	1.00	1.367	2.217
6.7	1.00	1.357	2.192
6.8	1.00	1.342	2.151
6.9	1.00	1.322	2.094
7.0	1.00	1.296	2.018
7.1	1.00	1.098	1.726
7.2	1.00	1.224	1.811
7.3	1.00	1.177	1.041
7.4	1.00	1.123	0.950
7.5	1.00	1.061	1.372
7.6	1.00	0.992	1.203
7.7	1.00	0.917	1.031
7.8	1.00	0.836	0.862
7.9	1.00	0.754	0.702
8.0	1.00	0.670	0.557
8.1	1.00	0.510	0.388
8.2	1.00	0.509	0.324
8.3	1.00	0.436	0.148
8.4	1.00	0.369	0.106
8.5	1.00	0.309	0.121
8.6	1.00	0.257	0.084
8.7	1.00	0.211	0.057
8.8	1.00	0.173	0.038
8.9	1.00	0.141	0.025
9.0	1.00	0.114	0.017
9.1	1.00	0.080	0.010
9.2	1.00	0.074	0.007
9.3	1.00	0.060	0.003
9.4	1.00	0.048	0.002
9.5	1.00	0.038	0.002
9.6	1.00	0.030	0.001
9.7	1.00	0.024	0.001
9.8	1.00	0.019	0.001
9.9	1.00	0.015	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 20 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.998	0.952
3.1	0.984	1.003	0.946
3.2	0.987	1.008	0.937
3.3	0.990	1.014	0.926
3.4	0.992	1.021	0.911
3.5	0.994	1.028	0.894
3.6	0.995	1.036	0.873
3.7	1.00	1.046	0.849
3.8	1.00	1.058	0.821
3.9	1.00	0.967	0.656
4.0	1.00	1.089	0.756
4.1	1.00	1.109	0.719
4.2	1.00	1.132	0.681
4.3	1.00	1.158	0.643
4.4	1.00	1.188	0.605
4.5	1.00	1.221	0.570
4.6	1.00	1.257	0.537
4.7	1.00	1.295	0.508
4.8	1.00	1.335	0.484
4.9	1.00	1.302	0.417
5.0	1.00	1.413	0.447
5.1	1.00	1.450	0.434
5.2	1.00	1.484	0.424
5.3	1.00	1.515	0.416
5.4	1.00	1.542	0.410
5.5	1.00	1.565	0.406
5.6	1.00	1.584	0.402
5.7	1.00	1.599	0.399
5.8	1.00	1.610	0.396
5.9	1.00	1.605	0.385
6.0	1.00	1.621	0.389
6.1	1.00	1.621	0.385
6.2	1.00	1.617	0.380
6.3	1.00	1.609	0.373
6.4	1.00	1.596	0.365
6.5	1.00	1.579	0.356
6.6	1.00	1.556	0.345
6.7	1.00	1.528	0.331
6.8	1.00	1.492	0.315
6.9	1.00	1.469	0.312
7.0	1.00	1.398	0.276
7.1	1.00	1.338	0.252
7.2	1.00	1.269	0.227
7.3	1.00	1.192	0.200
7.4	1.00	1.106	0.172
7.5	1.00	1.015	0.145
7.6	1.00	0.920	0.119
7.7	1.00	0.822	0.095
7.8	1.00	0.725	0.074
7.9	1.00	0.676	0.072
8.0	1.00	0.543	0.041
8.1	1.00	0.462	0.030
8.2	1.00	0.389	0.021
8.3	1.00	0.324	0.015
8.4	1.00	0.268	0.010
8.5	1.00	0.220	0.007
8.6	1.00	0.179	0.005
8.7	1.00	0.146	0.003
8.8	1.00	0.118	0.002
8.9	1.00	0.106	0.002
9.0	1.00	0.076	0.001
9.1	1.00	0.061	0.001
9.2	1.00	0.049	0.000
9.3	1.00	0.039	0.000
9.4	1.00	0.031	0.000
9.5	1.00	0.025	0.000
9.6	1.00	0.020	0.000
9.7	1.00	0.016	0.000
9.8	1.00	0.013	0.000
9.9	1.00	0.011	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 21 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.983	0.952
3.1	0.984	0.985	0.946
3.2	0.987	0.986	0.937
3.3	0.990	0.987	0.925
3.4	0.992	0.987	0.911
3.5	0.994	0.986	0.893
3.6	0.995	0.985	0.872
3.7	1.00	0.983	0.847
3.8	1.00	0.980	0.818
3.9	1.00	0.976	0.785
4.0	1.00	0.972	0.748
4.1	1.00	0.966	0.708
4.2	1.00	0.959	0.666
4.3	1.00	0.952	0.622
4.4	1.00	0.943	0.577
4.5	1.00	0.933	0.534
4.6	1.00	0.922	0.491
4.7	1.00	0.911	0.452
4.8	1.00	0.899	0.415
4.9	1.00	0.887	0.382
5.0	1.00	0.875	0.356
5.1	1.00	0.863	0.326
5.2	1.00	0.852	0.304
5.3	1.00	0.842	0.284
5.4	1.00	0.833	0.268
5.5	1.00	0.824	0.254
5.6	1.00	0.817	0.242
5.7	1.00	0.810	0.232
5.8	1.00	0.803	0.223
5.9	1.00	0.796	0.216
6.0	1.00	0.790	0.251
6.1	1.00	0.783	0.203
6.2	1.00	0.776	0.198
6.3	1.00	0.768	0.192
6.4	1.00	0.758	0.186
6.5	1.00	0.748	0.180
6.6	1.00	0.735	0.173
6.7	1.00	0.720	0.166
6.8	1.00	0.702	0.157
6.9	1.00	0.680	0.147
7.0	1.00	0.655	0.187
7.1	1.00	0.627	0.125
7.2	1.00	0.594	0.112
7.3	1.00	0.558	0.098
7.4	1.00	0.517	0.085
7.5	1.00	0.475	0.071
7.6	1.00	0.430	0.058
7.7	1.00	0.384	0.047
7.8	1.00	0.339	0.036
7.9	1.00	0.295	0.028
8.0	1.00	0.254	0.026
8.1	1.00	0.216	0.015
8.2	1.00	0.181	0.010
8.3	1.00	0.151	0.007
8.4	1.00	0.125	0.005
8.5	1.00	0.103	0.003
8.6	1.00	0.084	0.002
8.7	1.00	0.068	0.001
8.8	1.00	0.055	0.001
8.9	1.00	0.044	0.001
9.0	1.00	0.036	0.000
9.1	1.00	0.029	0.000
9.2	1.00	0.023	0.000
9.3	1.00	0.018	0.000
9.4	1.00	0.015	0.000
9.5	1.00	0.012	0.000
9.6	1.00	0.009	0.000
9.7	1.00	0.007	0.000
9.8	1.00	0.006	0.000
9.9	1.00	0.005	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 22 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.974	0.952
3.1	0.984	0.974	0.945
3.2	0.987	0.973	0.936
3.3	0.990	0.970	0.925
3.4	0.992	0.966	0.910
3.5	0.994	0.961	0.892
3.6	0.995	0.953	0.871
3.7	1.00	0.944	0.845
3.8	1.00	0.932	0.815
3.9	1.00	0.917	0.781
4.0	1.00	0.899	0.743
4.1	1.00	0.878	0.701
4.2	1.00	0.853	0.656
4.3	1.00	0.824	0.609
4.4	1.00	0.792	0.560
4.5	1.00	0.755	0.511
4.6	1.00	0.715	0.463
4.7	1.00	0.673	0.417
4.8	1.00	0.629	0.373
4.9	1.00	0.585	0.331
5.0	1.00	0.542	0.294
5.1	1.00	0.500	0.260
5.2	1.00	0.461	0.230
5.3	1.00	0.425	0.203
5.4	1.00	0.393	0.180
5.5	1.00	0.365	0.160
5.6	1.00	0.340	0.143
5.7	1.00	0.319	0.129
5.8	1.00	0.301	0.117
5.9	1.00	0.286	0.107
6.0	1.00	0.273	0.099
6.1	1.00	0.262	0.092
6.2	1.00	0.253	0.086
6.3	1.00	0.244	0.081
6.4	1.00	0.237	0.076
6.5	1.00	0.230	0.072
6.6	1.00	0.223	0.068
6.7	1.00	0.216	0.064
6.8	1.00	0.209	0.059
6.9	1.00	0.201	0.055
7.0	1.00	0.193	0.051
7.1	1.00	0.184	0.046
7.2	1.00	0.173	0.041
7.3	1.00	0.162	0.036
7.4	1.00	0.150	0.031
7.5	1.00	0.138	0.026
7.6	1.00	0.124	0.021
7.7	1.00	0.111	0.017
7.8	1.00	0.098	0.013
7.9	1.00	0.085	0.010
8.0	1.00	0.073	0.007
8.1	1.00	0.062	0.005
8.2	1.00	0.052	0.004
8.3	1.00	0.044	0.003
8.4	1.00	0.036	0.002
8.5	1.00	0.030	0.001
8.6	1.00	0.024	0.001
8.7	1.00	0.020	0.001
8.8	1.00	0.016	0.000
8.9	1.00	0.013	0.000
9.0	1.00	0.010	0.000
9.1	1.00	0.008	0.000
9.2	1.00	0.007	0.000
9.3	1.00	0.005	0.000
9.4	1.00	0.004	0.000
9.5	1.00	0.003	0.000
9.6	1.00	0.003	0.000
9.7	1.00	0.002	0.000
9.8	1.00	0.002	0.000
9.9	1.00	0.001	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 23 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.012	0.954
3.1	0.984	1.021	0.948
3.2	0.987	1.031	0.939
3.3	0.990	1.042	0.929
3.4	0.992	1.054	0.916
3.5	0.994	1.070	0.901
3.6	0.995	1.088	0.882
3.7	1.00	1.110	0.862
3.8	1.00	1.136	0.839
3.9	1.00	1.168	0.814
4.0	1.00	1.205	0.788
4.1	1.00	1.249	0.762
4.2	1.00	1.300	0.737
4.3	1.00	1.358	0.714
4.4	1.00	1.424	0.695
4.5	1.00	1.495	0.681
4.6	1.00	1.573	0.672
4.7	1.00	1.653	0.669
4.8	1.00	1.736	0.670
4.9	1.00	1.818	0.676
5.0	1.00	1.897	0.707
5.1	1.00	1.972	0.698
5.2	1.00	2.040	0.712
5.3	1.00	2.102	0.726
5.4	1.00	2.155	0.739
5.5	1.00	2.201	0.751
5.6	1.00	2.239	0.761
5.7	1.00	2.269	0.769
5.8	1.00	2.292	0.775
5.9	1.00	2.309	0.778
6.0	1.00	2.319	1.010
6.1	1.00	2.323	0.777
6.2	1.00	2.320	0.771
6.3	1.00	2.312	0.763
6.4	1.00	2.297	0.751
6.5	1.00	2.275	0.734
6.6	1.00	2.244	0.713
6.7	1.00	2.205	0.688
6.8	1.00	2.157	0.657
6.9	1.00	2.097	0.620
7.0	1.00	2.025	0.848
7.1	1.00	1.941	0.531
7.2	1.00	1.844	0.479
7.3	1.00	1.735	0.423
7.4	1.00	1.614	0.366
7.5	1.00	1.484	0.310
7.6	1.00	1.347	0.255
7.7	1.00	1.207	0.205
7.8	1.00	1.067	0.160
7.9	1.00	0.931	0.122
8.0	1.00	0.802	0.125
8.1	1.00	0.684	0.066
8.2	1.00	0.576	0.047
8.3	1.00	0.481	0.032
8.4	1.00	0.398	0.022
8.5	1.00	0.327	0.015
8.6	1.00	0.267	0.010
8.7	1.00	0.217	0.007
8.8	1.00	0.176	0.004
8.9	1.00	0.142	0.003
9.0	1.00	0.114	0.002
9.1	1.00	0.091	0.001
9.2	1.00	0.073	0.001
9.3	1.00	0.058	0.000
9.4	1.00	0.047	0.000
9.5	1.00	0.037	0.000
9.6	1.00	0.030	0.000
9.7	1.00	0.024	0.000
9.8	1.00	0.019	0.000
9.9	1.00	0.015	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 24 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.989	0.953
3.1	0.984	0.992	0.947
3.2	0.987	0.995	0.939
3.3	0.990	0.998	0.928
3.4	0.992	1.000	0.914
3.5	0.994	1.003	0.898
3.6	0.995	1.005	0.878
3.7	1.00	1.008	0.855
3.8	1.00	1.011	0.829
3.9	1.00	1.015	0.800
4.0	1.00	1.019	0.768
4.1	1.00	1.023	0.734
4.2	1.00	1.028	0.700
4.3	1.00	1.034	0.664
4.4	1.00	1.040	0.630
4.5	1.00	1.047	0.597
4.6	1.00	1.055	0.567
4.7	1.00	1.063	0.539
4.8	1.00	1.071	0.515
4.9	1.00	1.079	0.495
5.0	1.00	1.086	0.489
5.1	1.00	1.093	0.463
5.2	1.00	1.099	0.451
5.3	1.00	1.105	0.441
5.4	1.00	1.109	0.433
5.5	1.00	1.112	0.426
5.6	1.00	1.115	0.420
5.7	1.00	1.116	0.415
5.8	1.00	1.116	0.410
5.9	1.00	1.115	0.405
6.0	1.00	1.112	0.506
6.1	1.00	1.108	0.395
6.2	1.00	1.102	0.389
6.3	1.00	1.094	0.382
6.4	1.00	1.084	0.374
6.5	1.00	1.071	0.364
6.6	1.00	1.055	0.353
6.7	1.00	1.035	0.339
6.8	1.00	1.011	0.323
6.9	1.00	0.982	0.305
7.0	1.00	0.948	0.404
7.1	1.00	0.908	0.260
7.2	1.00	0.862	0.234
7.3	1.00	0.811	0.207
7.4	1.00	0.754	0.179
7.5	1.00	0.693	0.152
7.6	1.00	0.629	0.125
7.7	1.00	0.564	0.100
7.8	1.00	0.498	0.078
7.9	1.00	0.435	0.060
8.0	1.00	0.375	0.060
8.1	1.00	0.319	0.032
8.2	1.00	0.269	0.023
8.3	1.00	0.224	0.016
8.4	1.00	0.186	0.011
8.5	1.00	0.153	0.007
8.6	1.00	0.125	0.005
8.7	1.00	0.101	0.003
8.8	1.00	0.082	0.002
8.9	1.00	0.066	0.001
9.0	1.00	0.053	0.001
9.1	1.00	0.043	0.001
9.2	1.00	0.034	0.000
9.3	1.00	0.027	0.000
9.4	1.00	0.022	0.000
9.5	1.00	0.017	0.000
9.6	1.00	0.014	0.000
9.7	1.00	0.011	0.000
9.8	1.00	0.009	0.000
9.9	1.00	0.007	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 25 - Foodchain Multipliers for Great Lakes Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.975	0.953
3.1	0.984	0.974	0.947
3.2	0.987	0.974	0.938
3.3	0.990	0.971	0.912
3.4	0.992	0.967	0.895
3.5	0.994	0.962	0.896
3.6	0.995	0.955	0.875
3.7	1.00	0.945	0.851
3.8	1.00	0.934	0.823
3.9	1.00	0.920	0.792
4.0	1.00	0.903	0.756
4.1	1.00	0.876	0.717
4.2	1.00	0.860	0.677
4.3	1.00	0.834	0.570
4.4	1.00	0.803	0.521
4.5	1.00	0.770	0.545
4.6	1.00	0.735	0.502
4.7	1.00	0.697	0.460
4.8	1.00	0.659	0.420
4.9	1.00	0.620	0.383
5.0	1.00	0.583	0.349
5.1	1.00	0.520	0.310
5.2	1.00	0.515	0.290
5.3	1.00	0.485	0.195
5.4	1.00	0.459	0.176
5.5	1.00	0.436	0.226
5.6	1.00	0.416	0.210
5.7	1.00	0.399	0.197
5.8	1.00	0.384	0.185
5.9	1.00	0.371	0.176
6.0	1.00	0.361	0.167
6.1	1.00	0.311	0.148
6.2	1.00	0.343	0.154
6.3	1.00	0.335	0.095
6.4	1.00	0.328	0.091
6.5	1.00	0.321	0.136
6.6	1.00	0.313	0.131
6.7	1.00	0.306	0.124
6.8	1.00	0.297	0.118
6.9	1.00	0.287	0.110
7.0	1.00	0.276	0.102
7.1	1.00	0.229	0.085
7.2	1.00	0.250	0.084
7.3	1.00	0.235	0.046
7.4	1.00	0.218	0.040
7.5	1.00	0.200	0.054
7.6	1.00	0.182	0.045
7.7	1.00	0.162	0.036
7.8	1.00	0.144	0.028
7.9	1.00	0.125	0.021
8.0	1.00	0.108	0.016
8.1	1.00	0.080	0.011
8.2	1.00	0.077	0.008
8.3	1.00	0.065	0.004
8.4	1.00	0.053	0.002
8.5	1.00	0.044	0.003
8.6	1.00	0.036	0.002
8.7	1.00	0.029	0.001
8.8	1.00	0.024	0.001
8.9	1.00	0.019	0.001
9.0	1.00	0.015	0.000
9.1	1.00	0.011	0.000
9.2	1.00	0.010	0.000
9.3	1.00	0.008	0.000
9.4	1.00	0.006	0.000
9.5	1.00	0.005	0.000
9.6	1.00	0.004	0.000
9.7	1.00	0.003	0.000
9.8	1.00	0.003	0.000
9.9	1.00	0.002	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 26 - Foodchain Multipliers for USEPA Default Scenario, Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.990	0.994
3.1	0.984	1.003	1.001
3.2	0.987	1.015	1.008
3.3	0.990	1.028	1.015
3.4	0.992	1.043	1.023
3.5	0.994	1.059	1.033
3.6	0.995	1.079	1.044
3.7	1.00	1.103	1.057
3.8	1.00	1.131	1.074
3.9	1.00	0.928	0.868
4.0	1.00	1.211	1.122
4.1	1.00	1.266	1.156
4.2	1.00	1.334	1.199
4.3	1.00	1.419	1.255
4.4	1.00	1.525	1.327
4.5	1.00	1.656	1.421
4.6	1.00	1.817	1.544
4.7	1.00	2.017	1.703
4.8	1.00	2.261	1.910
4.9	1.00	2.070	1.699
5.0	1.00	2.917	2.525
5.1	1.00	3.346	2.968
5.2	1.00	3.854	3.525
5.3	1.00	4.446	4.216
5.4	1.00	5.127	5.057
5.5	1.00	5.896	6.055
5.6	1.00	6.745	7.209
5.7	1.00	7.663	8.506
5.8	1.00	8.630	9.919
5.9	1.00	8.513	9.757
6.0	1.00	10.615	12.932
6.1	1.00	11.577	14.434
6.2	1.00	12.485	15.866
6.3	1.00	13.317	17.186
6.4	1.00	14.057	18.359
6.5	1.00	14.695	19.360
6.6	1.00	15.225	20.174
6.7	1.00	15.645	20.792
6.8	1.00	15.957	21.210
6.9	1.00	15.931	21.171
7.0	1.00	16.264	21.438
7.1	1.00	16.261	21.245
7.2	1.00	16.154	20.845
7.3	1.00	15.942	20.235
7.4	1.00	15.621	19.414
7.5	1.00	15.189	18.384
7.6	1.00	14.645	17.155
7.7	1.00	13.988	15.749
7.8	1.00	13.223	14.198
7.9	1.00	13.218	14.192
8.0	1.00	11.411	10.854
8.1	1.00	10.401	9.181
8.2	1.00	9.355	7.590
8.3	1.00	8.301	6.134
8.4	1.00	7.269	4.852
8.5	1.00	6.284	3.762
8.6	1.00	5.368	2.867
8.7	1.00	4.536	2.155
8.8	1.00	3.795	1.601
8.9	1.00	3.794	1.601
9.0	1.00	2.591	0.868
9.1	1.00	2.119	0.637
9.2	1.00	1.724	0.469
9.3	1.00	1.396	0.346
9.4	1.00	1.126	0.257
9.5	1.00	0.906	0.192
9.6	1.00	0.727	0.144
9.7	1.00	0.582	0.109
9.8	1.00	0.465	0.083
9.9	1.00	0.465	0.083

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 27 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.977	0.987
3.1	0.984	0.986	0.993
3.2	0.987	0.995	0.998
3.3	0.990	1.003	1.002
3.4	0.992	1.011	1.007
3.5	0.994	1.020	1.012
3.6	0.995	1.030	1.018
3.7	1.00	1.041	1.025
3.8	1.00	1.054	1.033
3.9	1.00	1.070	1.044
4.0	1.00	1.090	1.056
4.1	1.00	1.114	1.072
4.2	1.00	1.144	1.093
4.3	1.00	1.181	1.119
4.4	1.00	1.227	1.153
4.5	1.00	1.284	1.196
4.6	1.00	1.354	1.252
4.7	1.00	1.441	1.325
4.8	1.00	1.547	1.420
4.9	1.00	1.676	1.542
5.0	1.00	1.831	1.698
5.1	1.00	2.018	1.897
5.2	1.00	2.238	2.147
5.3	1.00	2.495	2.455
5.4	1.00	2.790	2.829
5.5	1.00	3.124	3.270
5.6	1.00	3.492	3.780
5.7	1.00	3.890	4.351
5.8	1.00	4.309	4.972
5.9	1.00	4.740	5.626
6.0	1.00	5.170	6.292
6.1	1.00	5.586	6.948
6.2	1.00	5.979	7.573
6.3	1.00	6.339	8.148
6.4	1.00	6.659	8.657
6.5	1.00	6.933	9.089
6.6	1.00	7.160	9.439
6.7	1.00	7.339	9.701
6.8	1.00	7.471	9.874
6.9	1.00	7.555	9.957
7.0	1.00	7.592	9.949
7.1	1.00	7.583	9.848
7.2	1.00	7.527	9.653
7.3	1.00	7.423	9.363
7.4	1.00	7.270	8.977
7.5	1.00	7.066	8.495
7.6	1.00	6.811	7.923
7.7	1.00	6.503	7.269
7.8	1.00	6.146	6.549
7.9	1.00	5.744	5.784
8.0	1.00	5.303	5.000
8.1	1.00	4.833	4.225
8.2	1.00	4.346	3.490
8.3	1.00	3.857	2.817
8.4	1.00	3.377	2.225
8.5	1.00	2.919	1.723
8.6	1.00	2.494	1.311
8.7	1.00	2.107	0.983
8.8	1.00	1.763	0.729
8.9	1.00	1.462	0.536
9.0	1.00	1.203	0.393
9.1	1.00	0.984	0.287
9.2	1.00	0.801	0.211
9.3	1.00	0.648	0.155
9.4	1.00	0.523	0.115
9.5	1.00	0.421	0.085
9.6	1.00	0.338	0.064
9.7	1.00	0.270	0.048
9.8	1.00	0.216	0.037
9.9	1.00	0.173	0.028

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 28 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.969	0.983
3.1	0.984	0.976	0.987
3.2	0.987	0.982	0.991
3.3	0.990	0.987	0.994
3.4	0.992	0.992	0.997
3.5	0.994	0.995	1.000
3.6	0.995	0.999	1.002
3.7	1.00	1.003	1.005
3.8	1.00	1.006	1.008
3.9	1.00	1.010	1.012
4.0	1.00	1.015	1.016
4.1	1.00	1.020	1.021
4.2	1.00	1.027	1.027
4.3	1.00	1.034	1.035
4.4	1.00	1.044	1.045
4.5	1.00	1.055	1.057
4.6	1.00	1.069	1.073
4.7	1.00	1.086	1.093
4.8	1.00	1.107	1.118
4.9	1.00	1.133	1.150
5.0	1.00	1.163	1.189
5.1	1.00	1.200	1.238
5.2	1.00	1.244	1.298
5.3	1.00	1.294	1.371
5.4	1.00	1.352	1.457
5.5	1.00	1.418	1.557
5.6	1.00	1.490	1.670
5.7	1.00	1.568	1.794
5.8	1.00	1.651	1.928
5.9	1.00	1.735	2.066
6.0	1.00	1.819	2.206
6.1	1.00	1.900	2.342
6.2	1.00	1.976	2.470
6.3	1.00	2.045	2.585
6.4	1.00	2.106	2.686
6.5	1.00	2.157	2.769
6.6	1.00	2.198	2.833
6.7	1.00	2.228	2.876
6.8	1.00	2.248	2.899
6.9	1.00	2.257	2.900
7.0	1.00	2.256	2.879
7.1	1.00	2.243	2.834
7.2	1.00	2.218	2.766
7.3	1.00	2.181	2.673
7.4	1.00	2.131	2.554
7.5	1.00	2.067	2.410
7.6	1.00	1.990	2.241
7.7	1.00	1.898	2.051
7.8	1.00	1.792	1.842
7.9	1.00	1.673	1.622
8.0	1.00	1.544	1.397
8.1	1.00	1.406	1.176
8.2	1.00	1.264	0.967
8.3	1.00	1.121	0.776
8.4	1.00	0.982	0.609
8.5	1.00	0.848	0.468
8.6	1.00	0.725	0.352
8.7	1.00	0.612	0.261
8.8	1.00	0.512	0.191
8.9	1.00	0.425	0.139
9.0	1.00	0.350	0.100
9.1	1.00	0.286	0.072
9.2	1.00	0.233	0.052
9.3	1.00	0.188	0.037
9.4	1.00	0.152	0.027
9.5	1.00	0.122	0.020
9.6	1.00	0.098	0.015
9.7	1.00	0.079	0.011
9.8	1.00	0.063	0.008
9.9	1.00	0.050	0.006

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 29 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0)

Log Kow	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.005	1.003
3.1	0.984	1.021	1.012
3.2	0.987	1.038	1.022
3.3	0.990	1.056	1.032
3.4	0.992	1.078	1.045
3.5	0.994	1.103	1.060
3.6	0.995	1.133	1.078
3.7	1.00	1.170	1.100
3.8	1.00	1.216	1.129
3.9	1.00	1.273	1.165
4.0	1.00	1.344	1.212
4.1	1.00	1.431	1.272
4.2	1.00	1.540	1.349
4.3	1.00	1.675	1.450
4.4	1.00	1.843	1.582
4.5	1.00	2.049	1.754
4.6	1.00	2.302	1.979
4.7	1.00	2.612	2.272
4.8	1.00	2.986	2.653
4.9	1.00	3.437	3.143
5.0	1.00	3.972	3.765
5.1	1.00	4.601	4.545
5.2	1.00	5.328	5.504
5.3	1.00	6.155	6.656
5.4	1.00	7.078	8.006
5.5	1.00	8.086	9.545
5.6	1.00	9.160	11.247
5.7	1.00	10.276	13.073
5.8	1.00	11.406	14.968
5.9	1.00	12.519	16.874
6.0	1.00	13.586	18.730
6.1	1.00	14.581	20.482
6.2	1.00	15.486	22.086
6.3	1.00	16.287	23.511
6.4	1.00	16.979	24.737
6.5	1.00	17.559	25.756
6.6	1.00	18.032	26.568
6.7	1.00	18.400	27.175
6.8	1.00	18.670	27.583
6.9	1.00	18.847	27.797
7.0	1.00	18.934	27.818
7.1	1.00	18.934	27.646
7.2	1.00	18.845	27.276
7.3	1.00	18.667	26.702
7.4	1.00	18.394	25.915
7.5	1.00	18.021	24.906
7.6	1.00	17.542	23.670
7.7	1.00	16.952	22.208
7.8	1.00	16.247	20.534
7.9	1.00	15.427	18.674
8.0	1.00	14.497	16.670
8.1	1.00	13.468	14.583
8.2	1.00	12.360	12.482
8.3	1.00	11.198	10.445
8.4	1.00	10.011	8.541
8.5	1.00	8.831	6.829
8.6	1.00	7.690	5.345
8.7	1.00	6.613	4.104
8.8	1.00	5.622	3.099
8.9	1.00	4.730	2.309
9.0	1.00	3.942	1.704
9.1	1.00	3.259	1.248
9.2	1.00	2.675	0.912
9.3	1.00	2.183	0.666
9.4	1.00	1.772	0.488
9.5	1.00	1.433	0.359
9.6	1.00	1.154	0.265
9.7	1.00	0.928	0.198
9.8	1.00	0.744	0.148
9.9	1.00	0.595	0.112

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 30 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.983	0.992
3.1	0.984	0.994	0.998
3.2	0.987	1.005	1.005
3.3	0.990	1.015	1.011
3.4	0.992	1.026	1.018
3.5	0.994	1.039	1.026
3.6	0.995	1.054	1.036
3.7	1.00	1.071	1.047
3.8	1.00	1.092	1.062
3.9	1.00	1.117	1.079
4.0	1.00	1.148	1.102
4.1	1.00	1.187	1.131
4.2	1.00	1.235	1.168
4.3	1.00	1.294	1.216
4.4	1.00	1.368	1.279
4.5	1.00	1.458	1.359
4.6	1.00	1.569	1.464
4.7	1.00	1.704	1.600
4.8	1.00	1.868	1.775
4.9	1.00	2.065	1.999
5.0	1.00	2.299	2.282
5.1	1.00	2.574	2.635
5.2	1.00	2.892	3.066
5.3	1.00	3.253	3.583
5.4	1.00	3.657	4.185
5.5	1.00	4.097	4.870
5.6	1.00	4.566	5.626
5.7	1.00	5.054	6.435
5.8	1.00	5.548	7.273
5.9	1.00	6.034	8.114
6.0	1.00	6.500	8.932
6.1	1.00	6.935	9.703
6.2	1.00	7.329	10.408
6.3	1.00	7.679	11.034
6.4	1.00	7.980	11.571
6.5	1.00	8.232	12.016
6.6	1.00	8.437	12.368
6.7	1.00	8.596	12.630
6.8	1.00	8.711	12.802
6.9	1.00	8.784	12.887
7.0	1.00	8.818	12.886
7.1	1.00	8.812	12.797
7.2	1.00	8.766	12.618
7.3	1.00	8.680	12.347
7.4	1.00	8.550	11.977
7.5	1.00	8.375	11.507
7.6	1.00	8.150	10.931
7.7	1.00	7.875	10.253
7.8	1.00	7.546	9.476
7.9	1.00	7.165	8.614
8.0	1.00	6.732	7.686
8.1	1.00	6.254	6.720
8.2	1.00	5.739	5.748
8.3	1.00	5.199	4.806
8.4	1.00	4.648	3.926
8.5	1.00	4.100	3.136
8.6	1.00	3.570	2.451
8.7	1.00	3.070	1.879
8.8	1.00	2.610	1.416
8.9	1.00	2.196	1.053
9.0	1.00	1.830	0.775
9.1	1.00	1.513	0.566
9.2	1.00	1.242	0.412
9.3	1.00	1.013	0.300
9.4	1.00	0.823	0.219
9.5	1.00	0.665	0.161
9.6	1.00	0.536	0.118
9.7	1.00	0.431	0.088
9.8	1.00	0.345	0.066
9.9	1.00	0.276	0.050

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 31 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.985
3.1	0.984	0.977	0.990
3.2	0.987	0.984	0.994
3.3	0.990	0.990	0.993
3.4	0.992	0.995	0.996
3.5	0.994	1.000	1.006
3.6	0.995	1.004	1.010
3.7	1.00	1.009	1.015
3.8	1.00	1.015	1.020
3.9	1.00	1.021	1.027
4.0	1.00	1.028	1.035
4.1	1.00	1.029	1.040
4.2	1.00	1.047	1.057
4.3	1.00	1.060	1.031
4.4	1.00	1.075	1.040
4.5	1.00	1.094	1.117
4.6	1.00	1.117	1.148
4.7	1.00	1.146	1.186
4.8	1.00	1.180	1.235
4.9	1.00	1.221	1.295
5.0	1.00	1.269	1.369
5.1	1.00	1.262	1.399
5.2	1.00	1.392	1.566
5.3	1.00	1.468	1.422
5.4	1.00	1.551	1.523
5.5	1.00	1.643	1.993
5.6	1.00	1.740	2.167
5.7	1.00	1.841	2.350
5.8	1.00	1.943	2.537
5.9	1.00	2.044	2.723
6.0	1.00	2.140	2.903
6.1	1.00	1.987	2.729
6.2	1.00	2.310	3.222
6.3	1.00	2.381	2.656
6.4	1.00	2.442	2.741
6.5	1.00	2.493	3.560
6.6	1.00	2.532	3.630
6.7	1.00	2.562	3.678
6.8	1.00	2.582	3.706
6.9	1.00	2.592	3.712
7.0	1.00	2.592	3.697
7.1	1.00	2.263	3.189
7.2	1.00	2.564	3.598
7.3	1.00	2.534	2.765
7.4	1.00	2.492	2.677
7.5	1.00	2.438	3.261
7.6	1.00	2.371	3.092
7.7	1.00	2.289	2.895
7.8	1.00	2.192	2.671
7.9	1.00	2.080	2.423
8.0	1.00	1.954	2.157
8.1	1.00	1.587	1.632
8.2	1.00	1.665	1.604
8.3	1.00	1.508	1.051
8.4	1.00	1.348	0.855
8.5	1.00	1.189	0.863
8.6	1.00	1.035	0.670
8.7	1.00	0.890	0.510
8.8	1.00	0.757	0.381
8.9	1.00	0.637	0.280
9.0	1.00	0.531	0.203
9.1	1.00	0.383	0.125
9.2	1.00	0.360	0.105
9.3	1.00	0.294	0.059
9.4	1.00	0.238	0.042
9.5	1.00	0.193	0.039
9.6	1.00	0.155	0.028
9.7	1.00	0.125	0.020
9.8	1.00	0.100	0.015
9.9	1.00	0.080	0.011

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 32 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.990	0.994
3.1	0.984	1.003	1.001
3.2	0.987	1.015	1.007
3.3	0.990	1.028	1.015
3.4	0.992	1.043	1.023
3.5	0.994	1.059	1.032
3.6	0.995	1.079	1.043
3.7	1.00	1.102	1.056
3.8	1.00	1.131	1.072
3.9	1.00	0.928	0.867
4.0	1.00	1.210	1.119
4.1	1.00	1.265	1.152
4.2	1.00	1.333	1.195
4.3	1.00	1.417	1.249
4.4	1.00	1.522	1.320
4.5	1.00	1.652	1.411
4.6	1.00	1.812	1.530
4.7	1.00	2.009	1.685
4.8	1.00	2.250	1.886
4.9	1.00	2.060	1.677
5.0	1.00	2.896	2.478
5.1	1.00	3.317	2.901
5.2	1.00	3.814	3.432
5.3	1.00	4.391	4.087
5.4	1.00	5.051	4.877
5.5	1.00	5.791	5.808
5.6	1.00	6.605	6.876
5.7	1.00	7.478	8.067
5.8	1.00	8.392	9.352
5.9	1.00	8.278	9.199
6.0	1.00	10.246	12.054
6.1	1.00	11.134	13.380
6.2	1.00	11.964	14.632
6.3	1.00	12.717	15.772
6.4	1.00	13.380	16.772
6.5	1.00	13.944	17.610
6.6	1.00	14.405	18.274
6.7	1.00	14.761	18.757
6.8	1.00	15.014	19.056
6.9	1.00	14.989	19.021
7.0	1.00	15.214	19.093
7.1	1.00	15.164	18.828
7.2	1.00	15.011	18.370
7.3	1.00	14.756	17.718
7.4	1.00	14.394	16.875
7.5	1.00	13.925	15.847
7.6	1.00	13.349	14.648
7.7	1.00	12.667	13.305
7.8	1.00	11.888	11.854
7.9	1.00	11.884	11.849
8.0	1.00	10.094	8.830
8.1	1.00	9.121	7.368
8.2	1.00	8.130	6.011
8.3	1.00	7.151	4.798
8.4	1.00	6.209	3.753
8.5	1.00	5.325	2.883
8.6	1.00	4.515	2.182
8.7	1.00	3.789	1.632
8.8	1.00	3.151	1.210
8.9	1.00	3.151	1.210
9.0	1.00	2.131	0.658
9.1	1.00	1.737	0.485
9.2	1.00	1.408	0.359
9.3	1.00	1.138	0.267
9.4	1.00	0.916	0.199
9.5	1.00	0.736	0.150
9.6	1.00	0.589	0.114
9.7	1.00	0.471	0.087
9.8	1.00	0.377	0.067
9.9	1.00	0.377	0.067

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 33 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.977	0.987
3.1	0.984	0.986	0.992
3.2	0.987	0.995	0.997
3.3	0.990	1.003	1.002
3.4	0.992	1.011	1.006
3.5	0.994	1.020	1.012
3.6	0.995	1.029	1.017
3.7	1.00	1.040	1.024
3.8	1.00	1.054	1.032
3.9	1.00	1.069	1.042
4.0	1.00	1.089	1.054
4.1	1.00	1.113	1.069
4.2	1.00	1.142	1.089
4.3	1.00	1.179	1.114
4.4	1.00	1.225	1.146
4.5	1.00	1.281	1.188
4.6	1.00	1.350	1.242
4.7	1.00	1.435	1.312
4.8	1.00	1.540	1.402
4.9	1.00	1.666	1.518
5.0	1.00	1.818	1.667
5.1	1.00	2.000	1.856
5.2	1.00	2.215	2.091
5.3	1.00	2.464	2.380
5.4	1.00	2.749	2.729
5.5	1.00	3.068	3.138
5.6	1.00	3.420	3.606
5.7	1.00	3.796	4.127
5.8	1.00	4.191	4.688
5.9	1.00	4.592	5.274
6.0	1.00	4.990	5.865
6.1	1.00	5.372	6.441
6.2	1.00	5.730	6.983
6.3	1.00	6.054	7.476
6.4	1.00	6.338	7.906
6.5	1.00	6.579	8.266
6.6	1.00	6.775	8.548
6.7	1.00	6.925	8.749
6.8	1.00	7.029	8.869
6.9	1.00	7.088	8.906
7.0	1.00	7.102	8.858
7.1	1.00	7.071	8.724
7.2	1.00	6.994	8.503
7.3	1.00	6.871	8.195
7.4	1.00	6.699	7.799
7.5	1.00	6.478	7.319
7.6	1.00	6.208	6.761
7.7	1.00	5.889	6.137
7.8	1.00	5.526	5.464
7.9	1.00	5.124	4.764
8.0	1.00	4.691	4.063
8.1	1.00	4.238	3.388
8.2	1.00	3.777	2.760
8.3	1.00	3.322	2.200
8.4	1.00	2.884	1.718
8.5	1.00	2.473	1.318
8.6	1.00	2.097	0.995
8.7	1.00	1.760	0.742
8.8	1.00	1.464	0.549
8.9	1.00	1.208	0.404
9.0	1.00	0.990	0.297
9.1	1.00	0.807	0.218
9.2	1.00	0.654	0.161
9.3	1.00	0.528	0.119
9.4	1.00	0.425	0.089
9.5	1.00	0.342	0.067
9.6	1.00	0.274	0.050
9.7	1.00	0.219	0.038
9.8	1.00	0.175	0.029
9.9	1.00	0.140	0.023

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 34 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.969	0.983
3.1	0.984	0.976	0.987
3.2	0.987	0.982	0.991
3.3	0.990	0.987	0.994
3.4	0.992	0.991	0.996
3.5	0.994	0.995	0.999
3.6	0.995	0.999	1.001
3.7	1.00	1.002	1.004
3.8	1.00	1.006	1.007
3.9	1.00	1.010	1.010
4.0	1.00	1.014	1.014
4.1	1.00	1.019	1.018
4.2	1.00	1.025	1.024
4.3	1.00	1.033	1.031
4.4	1.00	1.042	1.039
4.5	1.00	1.053	1.050
4.6	1.00	1.066	1.064
4.7	1.00	1.082	1.082
4.8	1.00	1.102	1.104
4.9	1.00	1.126	1.132
5.0	1.00	1.155	1.168
5.1	1.00	1.190	1.212
5.2	1.00	1.231	1.265
5.3	1.00	1.278	1.330
5.4	1.00	1.332	1.406
5.5	1.00	1.393	1.494
5.6	1.00	1.459	1.594
5.7	1.00	1.531	1.703
5.8	1.00	1.605	1.818
5.9	1.00	1.681	1.937
6.0	1.00	1.756	2.056
6.1	1.00	1.827	2.170
6.2	1.00	1.893	2.276
6.3	1.00	1.953	2.371
6.4	1.00	2.004	2.451
6.5	1.00	2.047	2.515
6.6	1.00	2.079	2.562
6.7	1.00	2.102	2.591
6.8	1.00	2.115	2.600
6.9	1.00	2.118	2.590
7.0	1.00	2.110	2.559
7.1	1.00	2.091	2.506
7.2	1.00	2.061	2.432
7.3	1.00	2.019	2.334
7.4	1.00	1.964	2.214
7.5	1.00	1.895	2.071
7.6	1.00	1.813	1.907
7.7	1.00	1.718	1.726
7.8	1.00	1.611	1.532
7.9	1.00	1.492	1.331
8.0	1.00	1.366	1.130
8.1	1.00	1.233	0.938
8.2	1.00	1.099	0.760
8.3	1.00	0.966	0.602
8.4	1.00	0.838	0.466
8.5	1.00	0.719	0.354
8.6	1.00	0.609	0.265
8.7	1.00	0.511	0.195
8.8	1.00	0.425	0.142
8.9	1.00	0.351	0.103
9.0	1.00	0.288	0.074
9.1	1.00	0.234	0.054
9.2	1.00	0.190	0.039
9.3	1.00	0.153	0.028
9.4	1.00	0.124	0.021
9.5	1.00	0.099	0.015
9.6	1.00	0.080	0.011
9.7	1.00	0.064	0.009
9.8	1.00	0.051	0.006
9.9	1.00	0.041	0.005

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 35 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0.001)

Log Kow	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.005	1.003
3.1	0.984	1.021	1.012
3.2	0.987	1.038	1.021
3.3	0.990	1.056	1.032
3.4	0.992	1.077	1.044
3.5	0.994	1.103	1.059
3.6	0.995	1.133	1.077
3.7	1.00	1.170	1.099
3.8	1.00	1.216	1.127
3.9	1.00	1.272	1.163
4.0	1.00	1.342	1.209
4.1	1.00	1.430	1.268
4.2	1.00	1.538	1.344
4.3	1.00	1.673	1.443
4.4	1.00	1.839	1.572
4.5	1.00	2.044	1.741
4.6	1.00	2.295	1.961
4.7	1.00	2.601	2.247
4.8	1.00	2.972	2.618
4.9	1.00	3.416	3.093
5.0	1.00	3.943	3.695
5.1	1.00	4.561	4.446
5.2	1.00	5.272	5.363
5.3	1.00	6.079	6.461
5.4	1.00	6.974	7.739
5.5	1.00	7.947	9.187
5.6	1.00	8.979	10.778
5.7	1.00	10.046	12.473
5.8	1.00	11.120	14.221
5.9	1.00	12.171	15.965
6.0	1.00	13.172	17.652
6.1	1.00	14.100	19.232
6.2	1.00	14.939	20.667
6.3	1.00	15.676	21.930
6.4	1.00	16.306	23.005
6.5	1.00	16.830	23.885
6.6	1.00	17.249	24.569
6.7	1.00	17.568	25.060
6.8	1.00	17.791	25.362
6.9	1.00	17.923	25.477
7.0	1.00	17.966	25.406
7.1	1.00	17.920	25.147
7.2	1.00	17.785	24.694
7.3	1.00	17.558	24.041
7.4	1.00	17.233	23.180
7.5	1.00	16.807	22.107
7.6	1.00	16.273	20.821
7.7	1.00	15.628	19.333
7.8	1.00	14.871	17.663
7.9	1.00	14.008	15.848
8.0	1.00	13.046	13.941
8.1	1.00	12.005	12.003
8.2	1.00	10.905	10.106
8.3	1.00	9.776	8.316
8.4	1.00	8.647	6.691
8.5	1.00	7.549	5.269
8.6	1.00	6.508	4.069
8.7	1.00	5.545	3.089
8.8	1.00	4.674	2.313
8.9	1.00	3.903	1.713
9.0	1.00	3.231	1.260
9.1	1.00	2.656	0.924
9.2	1.00	2.169	0.676
9.3	1.00	1.763	0.496
9.4	1.00	1.427	0.366
9.5	1.00	1.150	0.271
9.6	1.00	0.925	0.202
9.7	1.00	0.742	0.152
9.8	1.00	0.594	0.115
9.9	1.00	0.474	0.088

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 36 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.983	0.992
3.1	0.984	0.994	0.998
3.2	0.987	1.004	1.004
3.3	0.990	1.015	1.011
3.4	0.992	1.026	1.017
3.5	0.994	1.039	1.025
3.6	0.995	1.053	1.035
3.7	1.00	1.070	1.046
3.8	1.00	1.091	1.060
3.9	1.00	1.116	1.077
4.0	1.00	1.147	1.099
4.1	1.00	1.186	1.127
4.2	1.00	1.233	1.164
4.3	1.00	1.292	1.210
4.4	1.00	1.365	1.271
4.5	1.00	1.454	1.350
4.6	1.00	1.564	1.451
4.7	1.00	1.697	1.583
4.8	1.00	1.859	1.752
4.9	1.00	2.053	1.968
5.0	1.00	2.282	2.204
5.1	1.00	2.551	2.578
5.2	1.00	2.861	2.989
5.3	1.00	3.213	3.478
5.4	1.00	3.603	4.046
5.5	1.00	4.027	4.688
5.6	1.00	4.477	5.392
5.7	1.00	4.941	6.140
5.8	1.00	5.409	6.909
5.9	1.00	5.866	7.677
6.0	1.00	6.302	7.591
6.1	1.00	6.706	9.110
6.2	1.00	7.071	9.738
6.3	1.00	7.391	10.290
6.4	1.00	7.664	10.759
6.5	1.00	7.890	11.140
6.6	1.00	8.071	11.435
6.7	1.00	8.207	11.644
6.8	1.00	8.301	11.768
6.9	1.00	8.354	11.809
7.0	1.00	8.367	9.940
7.1	1.00	8.340	11.637
7.2	1.00	8.273	11.420
7.3	1.00	8.164	11.113
7.4	1.00	8.011	10.710
7.5	1.00	7.810	10.210
7.6	1.00	7.561	9.612
7.7	1.00	7.260	8.921
7.8	1.00	6.908	8.147
7.9	1.00	6.506	7.306
8.0	1.00	6.059	4.908
8.1	1.00	5.575	5.527
8.2	1.00	5.064	4.649
8.3	1.00	4.539	3.822
8.4	1.00	4.015	3.072
8.5	1.00	3.505	2.416
8.6	1.00	3.022	1.863
8.7	1.00	2.575	1.412
8.8	1.00	2.170	1.055
8.9	1.00	1.812	0.779
9.0	1.00	1.500	0.444
9.1	1.00	1.233	0.418
9.2	1.00	1.007	0.305
9.3	1.00	0.818	0.223
9.4	1.00	0.662	0.164
9.5	1.00	0.534	0.121
9.6	1.00	0.429	0.090
9.7	1.00	0.344	0.067
9.8	1.00	0.276	0.051
9.9	1.00	0.220	0.039

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 37 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.985
3.1	0.984	0.977	0.989
3.2	0.987	0.984	0.994
3.3	0.990	0.990	0.993
3.4	0.992	0.995	0.995
3.5	0.994	0.999	1.005
3.6	0.995	1.004	1.009
3.7	1.00	1.009	1.013
3.8	1.00	1.014	1.018
3.9	1.00	1.020	1.024
4.0	1.00	1.027	1.032
4.1	1.00	1.028	1.037
4.2	1.00	1.046	1.053
4.3	1.00	1.058	1.026
4.4	1.00	1.073	1.034
4.5	1.00	1.091	1.108
4.6	1.00	1.114	1.137
4.7	1.00	1.141	1.174
4.8	1.00	1.174	1.219
4.9	1.00	1.214	1.275
5.0	1.00	1.260	1.344
5.1	1.00	1.251	1.369
5.2	1.00	1.378	1.527
5.3	1.00	1.449	1.382
5.4	1.00	1.528	1.474
5.5	1.00	1.614	1.919
5.6	1.00	1.706	2.077
5.7	1.00	1.800	2.242
5.8	1.00	1.894	2.410
5.9	1.00	1.987	2.576
6.0	1.00	2.075	2.734
6.1	1.00	1.922	2.561
6.2	1.00	2.229	3.013
6.3	1.00	2.292	2.475
6.4	1.00	2.346	2.547
6.5	1.00	2.389	3.298
6.6	1.00	2.422	3.353
6.7	1.00	2.446	3.388
6.8	1.00	2.460	3.403
6.9	1.00	2.465	3.398
7.0	1.00	2.460	3.371
7.1	1.00	2.142	2.896
7.2	1.00	2.420	3.252
7.3	1.00	2.383	2.485
7.4	1.00	2.335	2.390
7.5	1.00	2.274	2.888
7.6	1.00	2.199	2.714
7.7	1.00	2.110	2.514
7.8	1.00	2.007	2.291
7.9	1.00	1.889	2.049
8.0	1.00	1.759	1.797
8.1	1.00	1.414	1.336
8.2	1.00	1.469	1.292
8.3	1.00	1.317	0.832
8.4	1.00	1.164	0.665
8.5	1.00	1.016	0.660
8.6	1.00	0.876	0.505
8.7	1.00	0.746	0.379
8.8	1.00	0.629	0.280
8.9	1.00	0.525	0.204
9.0	1.00	0.435	0.148
9.1	1.00	0.312	0.090
9.2	1.00	0.292	0.076
9.3	1.00	0.237	0.043
9.4	1.00	0.192	0.031
9.5	1.00	0.155	0.029
9.6	1.00	0.124	0.021
9.7	1.00	0.100	0.015
9.8	1.00	0.080	0.011
9.9	1.00	0.064	0.009

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 38 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.989	0.991
3.1	0.984	1.002	0.998
3.2	0.987	1.014	1.004
3.3	0.990	1.027	1.010
3.4	0.992	1.041	1.017
3.5	0.994	1.057	1.025
3.6	0.995	1.075	1.034
3.7	1.00	1.098	1.044
3.8	1.00	1.126	1.058
3.9	1.00	0.924	0.855
4.0	1.00	1.202	1.096
4.1	1.00	1.254	1.122
4.2	1.00	1.318	1.156
4.3	1.00	1.398	1.200
4.4	1.00	1.496	1.256
4.5	1.00	1.617	1.328
4.6	1.00	1.764	1.421
4.7	1.00	1.944	1.539
4.8	1.00	2.161	1.690
4.9	1.00	1.978	1.503
5.0	1.00	2.725	2.117
5.1	1.00	3.081	2.409
5.2	1.00	3.488	2.760
5.3	1.00	3.946	3.173
5.4	1.00	4.451	3.647
5.5	1.00	4.994	4.176
5.6	1.00	5.565	4.748
5.7	1.00	6.147	5.347
5.8	1.00	6.725	5.954
5.9	1.00	6.633	5.853
6.0	1.00	7.805	7.108
6.1	1.00	8.279	7.619
6.2	1.00	8.696	8.064
6.3	1.00	9.049	8.436
6.4	1.00	9.335	8.726
6.5	1.00	9.553	8.931
6.6	1.00	9.703	9.049
6.7	1.00	9.786	9.077
6.8	1.00	9.800	9.015
6.9	1.00	9.784	8.998
7.0	1.00	9.626	8.616
7.1	1.00	9.434	8.278
7.2	1.00	9.172	7.849
7.3	1.00	8.838	7.334
7.4	1.00	8.434	6.743
7.5	1.00	7.963	6.090
7.6	1.00	7.431	5.395
7.7	1.00	6.849	4.681
7.8	1.00	6.230	3.977
7.9	1.00	6.228	3.975
8.0	1.00	4.952	2.693
8.1	1.00	4.327	2.151
8.2	1.00	3.733	1.688
8.3	1.00	3.183	1.306
8.4	1.00	2.685	0.998
8.5	1.00	2.243	0.757
8.6	1.00	1.857	0.571
8.7	1.00	1.527	0.430
8.8	1.00	1.248	0.323
8.9	1.00	1.248	0.323
9.0	1.00	0.821	0.185
9.1	1.00	0.662	0.141
9.2	1.00	0.532	0.108
9.3	1.00	0.427	0.083
9.4	1.00	0.342	0.064
9.5	1.00	0.273	0.049
9.6	1.00	0.218	0.039
9.7	1.00	0.174	0.030
9.8	1.00	0.139	0.024
9.9	1.00	0.139	0.024

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 39 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.976	0.985
3.1	0.984	0.985	0.989
3.2	0.987	0.993	0.993
3.3	0.990	1.001	0.997
3.4	0.992	1.009	1.001
3.5	0.994	1.017	1.004
3.6	0.995	1.026	1.008
3.7	1.00	1.037	1.013
3.8	1.00	1.049	1.018
3.9	1.00	1.063	1.024
4.0	1.00	1.081	1.032
4.1	1.00	1.103	1.042
4.2	1.00	1.130	1.054
4.3	1.00	1.163	1.070
4.4	1.00	1.204	1.091
4.5	1.00	1.254	1.118
4.6	1.00	1.315	1.153
4.7	1.00	1.389	1.199
4.8	1.00	1.478	1.258
4.9	1.00	1.585	1.333
5.0	1.00	1.711	1.427
5.1	1.00	1.858	1.544
5.2	1.00	2.026	1.685
5.3	1.00	2.214	1.852
5.4	1.00	2.422	2.045
5.5	1.00	2.646	2.261
5.6	1.00	2.881	2.494
5.7	1.00	3.120	2.739
5.8	1.00	3.358	2.987
5.9	1.00	3.587	3.229
6.0	1.00	3.801	3.458
6.1	1.00	3.995	3.665
6.2	1.00	4.164	3.845
6.3	1.00	4.307	3.993
6.4	1.00	4.422	4.107
6.5	1.00	4.507	4.184
6.6	1.00	4.564	4.223
6.7	1.00	4.591	4.224
6.8	1.00	4.588	4.185
6.9	1.00	4.556	4.106
7.0	1.00	4.493	3.985
7.1	1.00	4.400	3.823
7.2	1.00	4.274	3.621
7.3	1.00	4.115	3.379
7.4	1.00	3.925	3.104
7.5	1.00	3.704	2.800
7.6	1.00	3.456	2.478
7.7	1.00	3.184	2.148
7.8	1.00	2.896	1.822
7.9	1.00	2.599	1.513
8.0	1.00	2.301	1.230
8.1	1.00	2.010	0.981
8.2	1.00	1.734	0.768
8.3	1.00	1.479	0.593
8.4	1.00	1.247	0.452
8.5	1.00	1.042	0.342
8.6	1.00	0.863	0.257
8.7	1.00	0.709	0.193
8.8	1.00	0.580	0.145
8.9	1.00	0.471	0.109
9.0	1.00	0.381	0.082
9.1	1.00	0.307	0.062
9.2	1.00	0.247	0.048
9.3	1.00	0.198	0.036
9.4	1.00	0.159	0.028
9.5	1.00	0.127	0.022
9.6	1.00	0.101	0.017
9.7	1.00	0.081	0.013
9.8	1.00	0.064	0.010
9.9	1.00	0.051	0.008

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 40 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.968	0.980
3.1	0.984	0.975	0.984
3.2	0.987	0.981	0.987
3.3	0.990	0.985	0.989
3.4	0.992	0.989	0.991
3.5	0.994	0.993	0.992
3.6	0.995	0.996	0.993
3.7	1.00	0.999	0.993
3.8	1.00	1.001	0.993
3.9	1.00	1.004	0.993
4.0	1.00	1.007	0.992
4.1	1.00	1.010	0.994
4.2	1.00	1.014	0.991
4.3	1.00	1.019	0.990
4.4	1.00	1.024	0.989
4.5	1.00	1.030	0.989
4.6	1.00	1.038	0.989
4.7	1.00	1.047	0.989
4.8	1.00	1.058	0.992
4.9	1.00	1.072	0.996
5.0	1.00	1.087	1.002
5.1	1.00	1.105	1.024
5.2	1.00	1.126	1.024
5.3	1.00	1.149	1.040
5.4	1.00	1.174	1.059
5.5	1.00	1.201	1.082
5.6	1.00	1.229	1.107
5.7	1.00	1.258	1.134
5.8	1.00	1.286	1.161
5.9	1.00	1.313	1.187
6.0	1.00	1.337	1.211
6.1	1.00	1.359	1.271
6.2	1.00	1.376	1.248
6.3	1.00	1.389	1.259
6.4	1.00	1.398	1.264
6.5	1.00	1.402	1.262
6.6	1.00	1.401	1.254
6.7	1.00	1.394	1.237
6.8	1.00	1.381	1.212
6.9	1.00	1.361	1.179
7.0	1.00	1.335	1.135
7.1	1.00	1.301	1.127
7.2	1.00	1.259	1.019
7.3	1.00	1.209	0.946
7.4	1.00	1.150	0.864
7.5	1.00	1.084	0.776
7.6	1.00	1.010	0.683
7.7	1.00	0.929	0.589
7.8	1.00	0.844	0.496
7.9	1.00	0.757	0.409
8.0	1.00	0.670	0.330
8.1	1.00	0.585	0.276
8.2	1.00	0.504	0.202
8.3	1.00	0.430	0.154
8.4	1.00	0.363	0.116
8.5	1.00	0.303	0.086
8.6	1.00	0.251	0.064
8.7	1.00	0.206	0.047
8.8	1.00	0.168	0.035
8.9	1.00	0.137	0.026
9.0	1.00	0.111	0.019
9.1	1.00	0.089	0.015
9.2	1.00	0.072	0.011
9.3	1.00	0.058	0.008
9.4	1.00	0.046	0.006
9.5	1.00	0.037	0.005
9.6	1.00	0.029	0.004
9.7	1.00	0.023	0.003
9.8	1.00	0.019	0.002
9.9	1.00	0.015	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 41 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0.01)

Log Kow	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	1.004	1.000
3.1	0.984	1.020	1.008
3.2	0.987	1.036	1.017
3.3	0.990	1.054	1.027
3.4	0.992	1.075	1.038
3.5	0.994	1.100	1.051
3.6	0.995	1.129	1.066
3.7	1.00	1.165	1.086
3.8	1.00	1.210	1.111
3.9	1.00	1.264	1.142
4.0	1.00	1.332	1.182
4.1	1.00	1.416	1.233
4.2	1.00	1.520	1.298
4.3	1.00	1.648	1.383
4.4	1.00	1.805	1.492
4.5	1.00	1.998	1.633
4.6	1.00	2.231	1.814
4.7	1.00	2.513	2.045
4.8	1.00	2.848	2.338
4.9	1.00	3.244	2.704
5.0	1.00	3.703	3.153
5.1	1.00	4.228	3.694
5.2	1.00	4.818	4.330
5.3	1.00	5.465	5.060
5.4	1.00	6.160	5.872
5.5	1.00	6.887	6.749
5.6	1.00	7.628	7.666
5.7	1.00	8.362	8.595
5.8	1.00	9.071	9.505
5.9	1.00	9.734	10.367
6.0	1.00	10.339	11.158
6.1	1.00	10.874	11.858
6.2	1.00	11.335	12.456
6.3	1.00	11.717	12.945
6.4	1.00	12.021	13.320
6.5	1.00	12.249	13.581
6.6	1.00	12.403	13.729
6.7	1.00	12.485	13.763
6.8	1.00	12.495	13.682
6.9	1.00	12.434	13.485
7.0	1.00	12.301	13.169
7.1	1.00	12.093	12.732
7.2	1.00	11.807	12.171
7.3	1.00	11.441	11.488
7.4	1.00	10.993	10.690
7.5	1.00	10.463	9.789
7.6	1.00	9.854	8.805
7.7	1.00	9.176	7.767
7.8	1.00	8.440	6.710
7.9	1.00	7.663	5.673
8.0	1.00	6.866	4.692
8.1	1.00	6.069	3.798
8.2	1.00	5.295	3.014
8.3	1.00	4.562	2.349
8.4	1.00	3.885	1.802
8.5	1.00	3.273	1.366
8.6	1.00	2.731	1.026
8.7	1.00	2.260	0.767
8.8	1.00	1.857	0.572
8.9	1.00	1.516	0.426
9.0	1.00	1.232	0.318
9.1	1.00	0.997	0.239
9.2	1.00	0.803	0.180
9.3	1.00	0.646	0.137
9.4	1.00	0.518	0.104
9.5	1.00	0.415	0.080
9.6	1.00	0.331	0.062
9.7	1.00	0.264	0.048
9.8	1.00	0.211	0.037
9.9	1.00	0.168	0.029

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 42 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.982	0.989
3.1	0.984	0.993	0.995
3.2	0.987	1.003	1.000
3.3	0.990	1.013	1.006
3.4	0.992	1.024	1.011
3.5	0.994	1.036	1.018
3.6	0.995	1.050	1.025
3.7	1.00	1.066	1.034
3.8	1.00	1.086	1.044
3.9	1.00	1.109	1.058
4.0	1.00	1.139	1.075
4.1	1.00	1.175	1.096
4.2	1.00	1.219	1.124
4.3	1.00	1.273	1.160
4.4	1.00	1.340	1.207
4.5	1.00	1.421	1.266
4.6	1.00	1.520	1.344
4.7	1.00	1.640	1.442
4.8	1.00	1.782	1.567
4.9	1.00	1.949	1.723
5.0	1.00	2.143	1.915
5.1	1.00	2.365	2.145
5.2	1.00	2.615	2.417
5.3	1.00	2.889	2.728
5.4	1.00	3.182	3.073
5.5	1.00	3.490	3.447
5.6	1.00	3.803	3.837
5.7	1.00	4.113	4.231
5.8	1.00	4.412	4.617
5.9	1.00	4.692	4.982
6.0	1.00	4.947	5.316
6.1	1.00	5.172	5.612
6.2	1.00	5.365	5.862
6.3	1.00	5.524	6.066
6.4	1.00	5.650	6.220
6.5	1.00	5.743	6.324
6.6	1.00	5.803	6.378
6.7	1.00	5.832	6.383
6.8	1.00	5.830	6.336
6.9	1.00	5.795	6.237
7.0	1.00	5.729	6.085
7.1	1.00	5.628	5.878
7.2	1.00	5.492	5.615
7.3	1.00	5.320	5.296
7.4	1.00	5.110	4.925
7.5	1.00	4.862	4.506
7.6	1.00	4.579	4.050
7.7	1.00	4.263	3.570
7.8	1.00	3.920	3.081
7.9	1.00	3.559	2.602
8.0	1.00	3.188	2.150
8.1	1.00	2.818	1.738
8.2	1.00	2.459	1.377
8.3	1.00	2.118	1.071
8.4	1.00	1.804	0.820
8.5	1.00	1.520	0.620
8.6	1.00	1.268	0.464
8.7	1.00	1.049	0.346
8.8	1.00	0.862	0.257
8.9	1.00	0.704	0.191
9.0	1.00	0.572	0.142
9.1	1.00	0.463	0.106
9.2	1.00	0.373	0.080
9.3	1.00	0.300	0.060
9.4	1.00	0.240	0.046
9.5	1.00	0.192	0.035
9.6	1.00	0.154	0.027
9.7	1.00	0.123	0.021
9.8	1.00	0.098	0.016
9.9	1.00	0.078	0.013

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 43 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.969	0.982
3.1	0.984	0.976	0.986
3.2	0.987	0.983	0.990
3.3	0.990	0.988	0.988
3.4	0.992	0.993	0.989
3.5	0.994	0.997	0.997
3.6	0.995	1.001	0.999
3.7	1.00	1.005	1.001
3.8	1.00	1.009	1.004
3.9	1.00	1.014	1.006
4.0	1.00	1.019	1.009
4.1	1.00	1.018	1.008
4.2	1.00	1.033	1.017
4.3	1.00	1.043	0.984
4.4	1.00	1.054	0.983
4.5	1.00	1.067	1.041
4.6	1.00	1.083	1.054
4.7	1.00	1.102	1.071
4.8	1.00	1.125	1.092
4.9	1.00	1.152	1.119
5.0	1.00	1.183	1.152
5.1	1.00	1.160	1.143
5.2	1.00	1.259	1.239
5.3	1.00	1.303	1.093
5.4	1.00	1.350	1.128
5.5	1.00	1.399	1.414
5.6	1.00	1.449	1.480
5.7	1.00	1.498	1.546
5.8	1.00	1.545	1.609
5.9	1.00	1.589	1.669
6.0	1.00	1.628	1.722
6.1	1.00	1.482	1.570
6.2	1.00	1.691	1.805
6.3	1.00	1.713	1.453
6.4	1.00	1.729	1.465
6.5	1.00	1.739	1.858
6.6	1.00	1.742	1.855
6.7	1.00	1.738	1.841
6.8	1.00	1.728	1.815
6.9	1.00	1.710	1.777
7.0	1.00	1.684	1.725
7.1	1.00	1.445	1.443
7.2	1.00	1.606	1.580
7.3	1.00	1.553	1.170
7.4	1.00	1.489	1.084
7.5	1.00	1.416	1.255
7.6	1.00	1.332	1.124
7.7	1.00	1.239	0.987
7.8	1.00	1.139	0.848
7.9	1.00	1.033	0.713
8.0	1.00	0.925	0.585
8.1	1.00	0.715	0.404
8.2	1.00	0.713	0.369
8.3	1.00	0.614	0.224
8.4	1.00	0.523	0.169
8.5	1.00	0.441	0.161
8.6	1.00	0.368	0.119
8.7	1.00	0.304	0.087
8.8	1.00	0.250	0.063
8.9	1.00	0.204	0.046
9.0	1.00	0.166	0.034
9.1	1.00	0.117	0.021
9.2	1.00	0.108	0.018
9.3	1.00	0.087	0.011
9.4	1.00	0.070	0.008
9.5	1.00	0.056	0.008
9.6	1.00	0.045	0.006
9.7	1.00	0.036	0.004
9.8	1.00	0.028	0.003
9.9	1.00	0.023	0.003

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 44 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.982	0.968
3.1	0.984	0.992	0.969
3.2	0.987	1.002	0.968
3.3	0.990	1.011	0.966
3.4	0.992	1.022	0.962
3.5	0.994	1.033	0.957
3.6	0.995	1.045	0.951
3.7	1.00	1.060	0.942
3.8	1.00	1.077	0.932
3.9	1.00	0.884	0.753
4.0	1.00	1.123	0.908
4.1	1.00	1.152	0.893
4.2	1.00	1.188	0.878
4.3	1.00	1.230	0.863
4.4	1.00	1.278	0.848
4.5	1.00	1.334	0.835
4.6	1.00	1.398	0.823
4.7	1.00	1.469	0.815
4.8	1.00	1.546	0.810
4.9	1.00	1.415	0.718
5.0	1.00	1.712	0.809
5.1	1.00	1.798	0.814
5.2	1.00	1.882	0.820
5.3	1.00	1.961	0.828
5.4	1.00	2.035	0.837
5.5	1.00	2.102	0.845
5.6	1.00	2.161	0.853
5.7	1.00	2.211	0.859
5.8	1.00	2.251	0.864
5.9	1.00	2.221	0.846
6.0	1.00	2.307	0.867
6.1	1.00	2.323	0.865
6.2	1.00	2.330	0.861
6.3	1.00	2.329	0.854
6.4	1.00	2.320	0.843
6.5	1.00	2.303	0.829
6.6	1.00	2.276	0.812
6.7	1.00	2.239	0.789
6.8	1.00	2.191	0.762
6.9	1.00	2.188	0.760
7.0	1.00	2.060	0.692
7.1	1.00	1.974	0.649
7.2	1.00	1.876	0.601
7.3	1.00	1.764	0.549
7.4	1.00	1.641	0.494
7.5	1.00	1.508	0.437
7.6	1.00	1.368	0.381
7.7	1.00	1.224	0.326
7.8	1.00	1.082	0.276
7.9	1.00	1.081	0.276
8.0	1.00	0.812	0.189
8.1	1.00	0.692	0.154
8.2	1.00	0.583	0.124
8.3	1.00	0.486	0.100
8.4	1.00	0.402	0.080
8.5	1.00	0.330	0.064
8.6	1.00	0.270	0.051
8.7	1.00	0.219	0.040
8.8	1.00	0.177	0.032
8.9	1.00	0.177	0.032
9.0	1.00	0.115	0.020
9.1	1.00	0.092	0.016
9.2	1.00	0.074	0.013
9.3	1.00	0.059	0.010
9.4	1.00	0.047	0.008
9.5	1.00	0.037	0.006
9.6	1.00	0.030	0.005
9.7	1.00	0.024	0.004
9.8	1.00	0.019	0.003
9.9	1.00	0.019	0.003

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 45 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.968	0.961
3.1	0.984	0.975	0.961
3.2	0.987	0.981	0.958
3.3	0.990	0.986	0.954
3.4	0.992	0.990	0.947
3.5	0.994	0.994	0.938
3.6	0.995	0.997	0.927
3.7	1.00	1.000	0.914
3.8	1.00	1.004	0.897
3.9	1.00	1.007	0.877
4.0	1.00	1.010	0.855
4.1	1.00	1.014	0.829
4.2	1.00	1.018	0.801
4.3	1.00	1.023	0.770
4.4	1.00	1.029	0.738
4.5	1.00	1.035	0.704
4.6	1.00	1.042	0.671
4.7	1.00	1.049	0.638
4.8	1.00	1.058	0.607
4.9	1.00	1.066	0.578
5.0	1.00	1.075	0.552
5.1	1.00	1.084	0.529
5.2	1.00	1.093	0.509
5.3	1.00	1.101	0.491
5.4	1.00	1.108	0.476
5.5	1.00	1.114	0.463
5.6	1.00	1.119	0.453
5.7	1.00	1.122	0.443
5.8	1.00	1.124	0.435
5.9	1.00	1.125	0.428
6.0	1.00	1.124	0.421
6.1	1.00	1.121	0.414
6.2	1.00	1.116	0.408
6.3	1.00	1.109	0.401
6.4	1.00	1.099	0.393
6.5	1.00	1.086	0.384
6.6	1.00	1.070	0.374
6.7	1.00	1.050	0.362
6.8	1.00	1.026	0.348
6.9	1.00	0.996	0.332
7.0	1.00	0.962	0.314
7.1	1.00	0.921	0.294
7.2	1.00	0.874	0.272
7.3	1.00	0.821	0.248
7.4	1.00	0.764	0.222
7.5	1.00	0.701	0.197
7.6	1.00	0.636	0.171
7.7	1.00	0.569	0.146
7.8	1.00	0.503	0.123
7.9	1.00	0.438	0.102
8.0	1.00	0.378	0.084
8.1	1.00	0.321	0.068
8.2	1.00	0.271	0.055
8.3	1.00	0.226	0.044
8.4	1.00	0.187	0.035
8.5	1.00	0.153	0.028
8.6	1.00	0.125	0.022
8.7	1.00	0.102	0.018
8.8	1.00	0.082	0.014
8.9	1.00	0.066	0.011
9.0	1.00	0.053	0.009
9.1	1.00	0.043	0.007
9.2	1.00	0.034	0.006
9.3	1.00	0.027	0.004
9.4	1.00	0.022	0.003
9.5	1.00	0.017	0.003
9.6	1.00	0.014	0.002
9.7	1.00	0.011	0.002
9.8	1.00	0.009	0.001
9.9	1.00	0.007	0.001

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 46 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.960	0.957
3.1	0.984	0.965	0.956
3.2	0.987	0.969	0.952
3.3	0.990	0.971	0.946
3.4	0.992	0.971	0.938
3.5	0.994	0.970	0.927
3.6	0.995	0.968	0.913
3.7	1.00	0.964	0.896
3.8	1.00	0.958	0.875
3.9	1.00	0.951	0.851
4.0	1.00	0.941	0.822
4.1	1.00	0.929	0.790
4.2	1.00	0.914	0.753
4.3	1.00	0.896	0.713
4.4	1.00	0.875	0.670
4.5	1.00	0.850	0.624
4.6	1.00	0.822	0.577
4.7	1.00	0.791	0.530
4.8	1.00	0.757	0.483
4.9	1.00	0.721	0.437
5.0	1.00	0.683	0.394
5.1	1.00	0.645	0.354
5.2	1.00	0.607	0.317
5.3	1.00	0.571	0.284
5.4	1.00	0.537	0.254
5.5	1.00	0.505	0.229
5.6	1.00	0.477	0.207
5.7	1.00	0.452	0.188
5.8	1.00	0.431	0.172
5.9	1.00	0.412	0.158
6.0	1.00	0.395	0.147
6.1	1.00	0.381	0.137
6.2	1.00	0.369	0.129
6.3	1.00	0.358	0.122
6.4	1.00	0.348	0.115
6.5	1.00	0.338	0.110
6.6	1.00	0.328	0.104
6.7	1.00	0.319	0.099
6.8	1.00	0.309	0.093
6.9	1.00	0.298	0.088
7.0	1.00	0.286	0.082
7.1	1.00	0.272	0.076
7.2	1.00	0.258	0.069
7.3	1.00	0.241	0.063
7.4	1.00	0.224	0.056
7.5	1.00	0.205	0.049
7.6	1.00	0.186	0.042
7.7	1.00	0.166	0.035
7.8	1.00	0.147	0.029
7.9	1.00	0.128	0.024
8.0	1.00	0.110	0.020
8.1	1.00	0.094	0.016
8.2	1.00	0.079	0.012
8.3	1.00	0.066	0.010
8.4	1.00	0.054	0.008
8.5	1.00	0.045	0.006
8.6	1.00	0.036	0.005
8.7	1.00	0.030	0.004
8.8	1.00	0.024	0.003
8.9	1.00	0.019	0.002
9.0	1.00	0.015	0.002
9.1	1.00	0.012	0.001
9.2	1.00	0.010	0.001
9.3	1.00	0.008	0.001
9.4	1.00	0.006	0.001
9.5	1.00	0.005	0.001
9.6	1.00	0.004	0.000
9.7	1.00	0.003	0.000
9.8	1.00	0.003	0.000
9.9	1.00	0.002	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 47 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.995	0.974
3.1	0.984	1.009	0.977
3.2	0.987	1.023	0.978
3.3	0.990	1.038	0.978
3.4	0.992	1.054	0.978
3.5	0.994	1.073	0.977
3.6	0.995	1.095	0.975
3.7	1.00	1.122	0.973
3.8	1.00	1.154	0.970
3.9	1.00	1.192	0.968
4.0	1.00	1.238	0.967
4.1	1.00	1.294	0.967
4.2	1.00	1.360	0.970
4.3	1.00	1.438	0.975
4.4	1.00	1.528	0.985
4.5	1.00	1.631	1.001
4.6	1.00	1.747	1.022
4.7	1.00	1.874	1.049
4.8	1.00	2.011	1.082
4.9	1.00	2.154	1.121
5.0	1.00	2.301	1.163
5.1	1.00	2.446	1.208
5.2	1.00	2.587	1.253
5.3	1.00	2.720	1.297
5.4	1.00	2.842	1.338
5.5	1.00	2.950	1.376
5.6	1.00	3.045	1.408
5.7	1.00	3.125	1.435
5.8	1.00	3.191	1.457
5.9	1.00	3.243	1.473
6.0	1.00	3.281	1.483
6.1	1.00	3.307	1.487
6.2	1.00	3.321	1.485
6.3	1.00	3.323	1.477
6.4	1.00	3.313	1.463
6.5	1.00	3.291	1.441
6.6	1.00	3.256	1.412
6.7	1.00	3.207	1.375
6.8	1.00	3.142	1.328
6.9	1.00	3.061	1.272
7.0	1.00	2.962	1.206
7.1	1.00	2.844	1.131
7.2	1.00	2.707	1.046
7.3	1.00	2.552	0.954
7.4	1.00	2.379	0.856
7.5	1.00	2.191	0.756
7.6	1.00	1.993	0.656
7.7	1.00	1.789	0.559
7.8	1.00	1.585	0.469
7.9	1.00	1.386	0.388
8.0	1.00	1.197	0.316
8.1	1.00	1.021	0.255
8.2	1.00	0.862	0.204
8.3	1.00	0.720	0.162
8.4	1.00	0.597	0.128
8.5	1.00	0.491	0.101
8.6	1.00	0.401	0.080
8.7	1.00	0.326	0.063
8.8	1.00	0.264	0.049
8.9	1.00	0.213	0.039
9.0	1.00	0.171	0.031
9.1	1.00	0.138	0.024
9.2	1.00	0.110	0.019
9.3	1.00	0.088	0.015
9.4	1.00	0.070	0.012
9.5	1.00	0.056	0.010
9.6	1.00	0.045	0.008
9.7	1.00	0.036	0.006
9.8	1.00	0.028	0.005
9.9	1.00	0.023	0.004

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 48 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.974	0.964
3.1	0.984	0.983	0.964
3.2	0.987	0.990	0.962
3.3	0.990	0.997	0.958
3.4	0.992	1.004	0.953
3.5	0.994	1.011	0.946
3.6	0.995	1.018	0.937
3.7	1.00	1.026	0.926
3.8	1.00	1.035	0.912
3.9	1.00	1.046	0.897
4.0	1.00	1.058	0.883
4.1	1.00	1.073	0.861
4.2	1.00	1.090	0.841
4.3	1.00	1.111	0.820
4.4	1.00	1.134	0.799
4.5	1.00	1.160	0.779
4.6	1.00	1.190	0.761
4.7	1.00	1.223	0.745
4.8	1.00	1.258	0.732
4.9	1.00	1.294	0.722
5.0	1.00	1.331	0.810
5.1	1.00	1.368	0.710
5.2	1.00	1.404	0.707
5.3	1.00	1.438	0.706
5.4	1.00	1.468	0.706
5.5	1.00	1.495	0.707
5.6	1.00	1.518	0.707
5.7	1.00	1.537	0.707
5.8	1.00	1.552	0.707
5.9	1.00	1.563	0.705
6.0	1.00	1.570	1.207
6.1	1.00	1.573	0.699
6.2	1.00	1.572	0.693
6.3	1.00	1.567	0.686
6.4	1.00	1.557	0.676
6.5	1.00	1.543	0.663
6.6	1.00	1.523	0.648
6.7	1.00	1.498	0.629
6.8	1.00	1.466	0.607
6.9	1.00	1.427	0.580
7.0	1.00	1.379	1.144
7.1	1.00	1.324	0.514
7.2	1.00	1.259	0.475
7.3	1.00	1.186	0.432
7.4	1.00	1.106	0.387
7.5	1.00	1.018	0.341
7.6	1.00	0.926	0.295
7.7	1.00	0.831	0.251
7.8	1.00	0.736	0.211
7.9	1.00	0.644	0.174
8.0	1.00	0.556	0.329
8.1	1.00	0.474	0.114
8.2	1.00	0.400	0.091
8.3	1.00	0.334	0.072
8.4	1.00	0.277	0.057
8.5	1.00	0.228	0.045
8.6	1.00	0.186	0.035
8.7	1.00	0.152	0.028
8.8	1.00	0.123	0.022
8.9	1.00	0.099	0.017
9.0	1.00	0.080	0.023
9.1	1.00	0.064	0.011
9.2	1.00	0.051	0.008
9.3	1.00	0.041	0.007
9.4	1.00	0.033	0.005
9.5	1.00	0.026	0.004
9.6	1.00	0.021	0.003
9.7	1.00	0.017	0.003
9.8	1.00	0.013	0.002
9.9	1.00	0.010	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 49 - Foodchain Multipliers for Warmwater Benthic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.961	0.957
3.1	0.984	0.966	0.955
3.2	0.987	0.970	0.952
3.3	0.990	0.972	0.942
3.4	0.992	0.973	0.932
3.5	0.994	0.973	0.927
3.6	0.995	0.971	0.914
3.7	1.00	0.967	0.897
3.8	1.00	0.963	0.877
3.9	1.00	0.956	0.853
4.0	1.00	0.948	0.826
4.1	1.00	0.930	0.792
4.2	1.00	0.925	0.761
4.3	1.00	0.909	0.699
4.4	1.00	0.891	0.656
4.5	1.00	0.871	0.643
4.6	1.00	0.848	0.601
4.7	1.00	0.822	0.558
4.8	1.00	0.794	0.517
4.9	1.00	0.765	0.477
5.0	1.00	0.735	0.439
5.1	1.00	0.671	0.388
5.2	1.00	0.676	0.372
5.3	1.00	0.648	0.299
5.4	1.00	0.623	0.274
5.5	1.00	0.599	0.295
5.6	1.00	0.578	0.276
5.7	1.00	0.560	0.259
5.8	1.00	0.544	0.245
5.9	1.00	0.529	0.233
6.0	1.00	0.517	0.223
6.1	1.00	0.451	0.189
6.2	1.00	0.495	0.206
6.3	1.00	0.486	0.159
6.4	1.00	0.477	0.153
6.5	1.00	0.467	0.185
6.6	1.00	0.457	0.178
6.7	1.00	0.446	0.170
6.8	1.00	0.434	0.162
6.9	1.00	0.421	0.154
7.0	1.00	0.406	0.144
7.1	1.00	0.340	0.115
7.2	1.00	0.368	0.123
7.3	1.00	0.346	0.088
7.4	1.00	0.322	0.078
7.5	1.00	0.296	0.086
7.6	1.00	0.269	0.074
7.7	1.00	0.242	0.062
7.8	1.00	0.214	0.051
7.9	1.00	0.187	0.042
8.0	1.00	0.161	0.034
8.1	1.00	0.120	0.022
8.2	1.00	0.116	0.021
8.3	1.00	0.097	0.013
8.4	1.00	0.080	0.010
8.5	1.00	0.066	0.010
8.6	1.00	0.054	0.008
8.7	1.00	0.044	0.006
8.8	1.00	0.036	0.005
8.9	1.00	0.029	0.004
9.0	1.00	0.023	0.003
9.1	1.00	0.016	0.002
9.2	1.00	0.015	0.002
9.3	1.00	0.012	0.001
9.4	1.00	0.009	0.001
9.5	1.00	0.008	0.001
9.6	1.00	0.006	0.001
9.7	1.00	0.005	0.001
9.8	1.00	0.004	0.000
9.9	1.00	0.003	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 50 - Foodchain Multipliers for USEPA Default Scenario, Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.976	0.994
3.1	0.984	0.986	1.001
3.2	0.987	0.994	1.008
3.3	0.990	1.002	1.015
3.4	0.992	1.010	1.023
3.5	0.994	1.018	1.032
3.6	0.995	1.028	1.043
3.7	1.00	1.038	1.055
3.8	1.00	1.051	1.071
3.9	1.00	0.848	0.865
4.0	1.00	1.085	1.115
4.1	1.00	1.108	1.145
4.2	1.00	1.137	1.182
4.3	1.00	1.172	1.229
4.4	1.00	1.215	1.288
4.5	1.00	1.270	1.362
4.6	1.00	1.336	1.453
4.7	1.00	1.419	1.567
4.8	1.00	1.519	1.708
4.9	1.00	1.328	1.497
5.0	1.00	1.790	2.096
5.1	1.00	1.966	2.355
5.2	1.00	2.176	2.668
5.3	1.00	2.420	3.040
5.4	1.00	2.701	3.476
5.5	1.00	3.017	3.976
5.6	1.00	3.367	4.538
5.7	1.00	3.745	5.154
5.8	1.00	4.143	5.812
5.9	1.00	4.026	5.650
6.0	1.00	4.960	7.181
6.1	1.00	5.356	7.851
6.2	1.00	5.729	8.484
6.3	1.00	6.071	9.061
6.4	1.00	6.374	9.570
6.5	1.00	6.635	10.001
6.6	1.00	6.850	10.346
6.7	1.00	7.020	10.604
6.8	1.00	7.144	10.771
6.9	1.00	7.118	10.732
7.0	1.00	7.258	10.832
7.1	1.00	7.249	10.723
7.2	1.00	7.195	10.520
7.3	1.00	7.095	10.219
7.4	1.00	6.949	9.820
7.5	1.00	6.754	9.323
7.6	1.00	6.509	8.732
7.7	1.00	6.215	8.057
7.8	1.00	5.874	7.310
7.9	1.00	5.869	7.304
8.0	1.00	5.068	5.690
8.1	1.00	4.619	4.873
8.2	1.00	4.154	4.089
8.3	1.00	3.686	3.365
8.4	1.00	3.227	2.718
8.5	1.00	2.790	2.160
8.6	1.00	2.383	1.693
8.7	1.00	2.013	1.313
8.8	1.00	1.684	1.010
8.9	1.00	1.684	1.010
9.0	1.00	1.150	0.591
9.1	1.00	0.941	0.451
9.2	1.00	0.765	0.345
9.3	1.00	0.620	0.265
9.4	1.00	0.500	0.204
9.5	1.00	0.402	0.158
9.6	1.00	0.323	0.122
9.7	1.00	0.258	0.095
9.8	1.00	0.207	0.074
9.9	1.00	0.206	0.074

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 51 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.973	0.987
3.1	0.984	0.981	0.993
3.2	0.987	0.989	0.997
3.3	0.990	0.995	1.002
3.4	0.992	1.002	1.007
3.5	0.994	1.008	1.012
3.6	0.995	1.015	1.018
3.7	1.00	1.023	1.025
3.8	1.00	1.032	1.033
3.9	1.00	1.042	1.042
4.0	1.00	1.055	1.054
4.1	1.00	1.070	1.069
4.2	1.00	1.089	1.088
4.3	1.00	1.112	1.112
4.4	1.00	1.141	1.142
4.5	1.00	1.177	1.180
4.6	1.00	1.221	1.227
4.7	1.00	1.275	1.288
4.8	1.00	1.341	1.364
4.9	1.00	1.421	1.460
5.0	1.00	1.518	1.579
5.1	1.00	1.634	1.727
5.2	1.00	1.772	1.909
5.3	1.00	1.932	2.128
5.4	1.00	2.116	2.389
5.5	1.00	2.324	2.693
5.6	1.00	2.554	3.038
5.7	1.00	2.802	3.420
5.8	1.00	3.063	3.831
5.9	1.00	3.331	4.260
6.0	1.00	3.599	4.695
6.1	1.00	3.858	5.120
6.2	1.00	4.103	5.522
6.3	1.00	4.326	5.891
6.4	1.00	4.524	6.215
6.5	1.00	4.694	6.489
6.6	1.00	4.834	6.709
6.7	1.00	4.944	6.871
6.8	1.00	5.023	6.975
6.9	1.00	5.071	7.019
7.0	1.00	5.091	7.003
7.1	1.00	5.080	6.925
7.2	1.00	5.038	6.785
7.3	1.00	4.966	6.581
7.4	1.00	4.861	6.312
7.5	1.00	4.723	5.978
7.6	1.00	4.551	5.583
7.7	1.00	4.344	5.132
7.8	1.00	4.105	4.636
7.9	1.00	3.836	4.108
8.0	1.00	3.541	3.565
8.1	1.00	3.227	3.029
8.2	1.00	2.902	2.517
8.3	1.00	2.574	2.048
8.4	1.00	2.254	1.632
8.5	1.00	1.949	1.278
8.6	1.00	1.664	0.984
8.7	1.00	1.406	0.749
8.8	1.00	1.176	0.564
8.9	1.00	0.976	0.423
9.0	1.00	0.803	0.316
9.1	1.00	0.657	0.236
9.2	1.00	0.534	0.176
9.3	1.00	0.433	0.132
9.4	1.00	0.349	0.100
9.5	1.00	0.281	0.076
9.6	1.00	0.225	0.058
9.7	1.00	0.180	0.044
9.8	1.00	0.144	0.034
9.9	1.00	0.115	0.027

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 52 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.971	0.983
3.1	0.984	0.979	0.988
3.2	0.987	0.986	0.991
3.3	0.990	0.992	0.994
3.4	0.992	0.997	0.997
3.5	0.994	1.002	1.000
3.6	0.995	1.008	1.003
3.7	1.00	1.013	1.006
3.8	1.00	1.020	1.009
3.9	1.00	1.027	1.013
4.0	1.00	1.036	1.017
4.1	1.00	1.047	1.023
4.2	1.00	1.060	1.030
4.3	1.00	1.076	1.040
4.4	1.00	1.095	1.052
4.5	1.00	1.119	1.067
4.6	1.00	1.149	1.088
4.7	1.00	1.186	1.116
4.8	1.00	1.231	1.152
4.9	1.00	1.285	1.199
5.0	1.00	1.351	1.261
5.1	1.00	1.430	1.341
5.2	1.00	1.523	1.441
5.3	1.00	1.632	1.567
5.4	1.00	1.757	1.721
5.5	1.00	1.898	1.903
5.6	1.00	2.053	2.115
5.7	1.00	2.221	2.353
5.8	1.00	2.398	2.612
5.9	1.00	2.580	2.886
6.0	1.00	2.761	3.165
6.1	1.00	2.937	3.439
6.2	1.00	3.102	3.700
6.3	1.00	3.253	3.939
6.4	1.00	3.386	4.151
6.5	1.00	3.500	4.329
6.6	1.00	3.593	4.471
6.7	1.00	3.666	4.574
6.8	1.00	3.717	4.639
6.9	1.00	3.747	4.663
7.0	1.00	3.756	4.646
7.1	1.00	3.744	4.588
7.2	1.00	3.711	4.487
7.3	1.00	3.655	4.342
7.4	1.00	3.576	4.153
7.5	1.00	3.473	3.920
7.6	1.00	3.345	3.645
7.7	1.00	3.193	3.333
7.8	1.00	3.016	2.990
7.9	1.00	2.818	2.628
8.0	1.00	2.601	2.258
8.1	1.00	2.370	1.894
8.2	1.00	2.131	1.550
8.3	1.00	1.891	1.237
8.4	1.00	1.655	0.964
8.5	1.00	1.431	0.735
8.6	1.00	1.222	0.548
8.7	1.00	1.033	0.402
8.8	1.00	0.864	0.290
8.9	1.00	0.716	0.207
9.0	1.00	0.590	0.146
9.1	1.00	0.482	0.103
9.2	1.00	0.392	0.072
9.3	1.00	0.318	0.051
9.4	1.00	0.256	0.036
9.5	1.00	0.206	0.026
9.6	1.00	0.165	0.018
9.7	1.00	0.132	0.013
9.8	1.00	0.106	0.010
9.9	1.00	0.085	0.007

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 53 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.983	1.003
3.1	0.984	0.993	1.012
3.2	0.987	1.003	1.021
3.3	0.990	1.014	1.031
3.4	0.992	1.024	1.043
3.5	0.994	1.037	1.058
3.6	0.995	1.050	1.075
3.7	1.00	1.067	1.096
3.8	1.00	1.087	1.122
3.9	1.00	1.111	1.154
4.0	1.00	1.141	1.194
4.1	1.00	1.178	1.245
4.2	1.00	1.223	1.308
4.3	1.00	1.280	1.387
4.4	1.00	1.349	1.486
4.5	1.00	1.435	1.609
4.6	1.00	1.541	1.763
4.7	1.00	1.669	1.954
4.8	1.00	1.825	2.190
4.9	1.00	2.012	2.479
5.0	1.00	2.235	2.831
5.1	1.00	2.496	3.253
5.2	1.00	2.798	3.752
5.3	1.00	3.142	4.332
5.4	1.00	3.525	4.993
5.5	1.00	3.944	5.727
5.6	1.00	4.390	6.524
5.7	1.00	4.853	7.364
5.8	1.00	5.323	8.224
5.9	1.00	5.785	9.079
6.0	1.00	6.228	9.905
6.1	1.00	6.641	10.678
6.2	1.00	7.016	11.381
6.3	1.00	7.348	12.002
6.4	1.00	7.634	12.533
6.5	1.00	7.874	12.972
6.6	1.00	8.068	13.318
6.7	1.00	8.219	13.573
6.8	1.00	8.328	13.739
6.9	1.00	8.397	13.818
7.0	1.00	8.429	13.811
7.1	1.00	8.423	13.716
7.2	1.00	8.379	13.532
7.3	1.00	8.296	13.253
7.4	1.00	8.171	12.876
7.5	1.00	8.004	12.396
7.6	1.00	7.789	11.810
7.7	1.00	7.526	11.117
7.8	1.00	7.212	10.322
7.9	1.00	6.847	9.438
8.0	1.00	6.434	8.483
8.1	1.00	5.977	7.483
8.2	1.00	5.485	6.472
8.3	1.00	4.969	5.485
8.4	1.00	4.442	4.554
8.5	1.00	3.918	3.708
8.6	1.00	3.412	2.966
8.7	1.00	2.934	2.335
8.8	1.00	2.494	1.814
8.9	1.00	2.098	1.395
9.0	1.00	1.749	1.066
9.1	1.00	1.446	0.811
9.2	1.00	1.187	0.617
9.3	1.00	0.968	0.469
9.4	1.00	0.786	0.357
9.5	1.00	0.636	0.273
9.6	1.00	0.512	0.210
9.7	1.00	0.412	0.162
9.8	1.00	0.330	0.125
9.9	1.00	0.264	0.097

Notes
Kow = n-octanol-water partition coefficient
Km = metabolic transformation rate constant
$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow
C = Celsius

Table 54 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, Km = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.977	0.992
3.1	0.984	0.987	0.998
3.2	0.987	0.995	1.004
3.3	0.990	1.003	1.011
3.4	0.992	1.012	1.018
3.5	0.994	1.021	1.026
3.6	0.995	1.031	1.035
3.7	1.00	1.042	1.046
3.8	1.00	1.056	1.060
3.9	1.00	1.072	1.076
4.0	1.00	1.092	1.097
4.1	1.00	1.117	1.124
4.2	1.00	1.147	1.157
4.3	1.00	1.184	1.199
4.4	1.00	1.231	1.252
4.5	1.00	1.287	1.319
4.6	1.00	1.357	1.404
4.7	1.00	1.442	1.512
4.8	1.00	1.545	1.647
4.9	1.00	1.669	1.815
5.0	1.00	1.816	2.023
5.1	1.00	1.989	2.276
5.2	1.00	2.189	2.580
5.3	1.00	2.416	2.937
5.4	1.00	2.670	3.348
5.5	1.00	2.946	3.810
5.6	1.00	3.241	4.314
5.7	1.00	3.548	4.849
5.8	1.00	3.858	5.399
5.9	1.00	4.164	5.949
6.0	1.00	4.456	6.481
6.1	1.00	4.729	6.980
6.2	1.00	4.977	7.435
6.3	1.00	5.196	7.837
6.4	1.00	5.384	8.181
6.5	1.00	5.542	8.464
6.6	1.00	5.669	8.688
6.7	1.00	5.767	8.851
6.8	1.00	5.838	8.956
6.9	1.00	5.882	9.004
7.0	1.00	5.900	8.995
7.1	1.00	5.892	8.928
7.2	1.00	5.859	8.800
7.3	1.00	5.799	8.611
7.4	1.00	5.710	8.356
7.5	1.00	5.592	8.032
7.6	1.00	5.441	7.637
7.7	1.00	5.257	7.172
7.8	1.00	5.037	6.639
7.9	1.00	4.781	6.048
8.0	1.00	4.492	5.412
8.1	1.00	4.173	4.748
8.2	1.00	3.830	4.079
8.3	1.00	3.469	3.428
8.4	1.00	3.101	2.819
8.5	1.00	2.736	2.269
8.6	1.00	2.382	1.790
8.7	1.00	2.048	1.387
8.8	1.00	1.741	1.059
8.9	1.00	1.465	0.799
9.0	1.00	1.221	0.598
9.1	1.00	1.009	0.445
9.2	1.00	0.828	0.330
9.3	1.00	0.676	0.246
9.4	1.00	0.549	0.183
9.5	1.00	0.444	0.137
9.6	1.00	0.358	0.103
9.7	1.00	0.287	0.078
9.8	1.00	0.230	0.059
9.9	1.00	0.184	0.046

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 55 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.974	0.985
3.1	0.984	0.982	0.990
3.2	0.987	0.990	0.994
3.3	0.990	0.997	0.993
3.4	0.992	1.004	0.996
3.5	0.994	1.011	1.006
3.6	0.995	1.018	1.010
3.7	1.00	1.027	1.015
3.8	1.00	1.036	1.021
3.9	1.00	1.048	1.028
4.0	1.00	1.062	1.037
4.1	1.00	1.077	1.045
4.2	1.00	1.100	1.064
4.3	1.00	1.126	1.039
4.4	1.00	1.157	1.053
4.5	1.00	1.197	1.141
4.6	1.00	1.244	1.183
4.7	1.00	1.303	1.240
4.8	1.00	1.373	1.312
4.9	1.00	1.458	1.406
5.0	1.00	1.559	1.525
5.1	1.00	1.661	1.644
5.2	1.00	1.814	1.858
5.3	1.00	1.970	1.727
5.4	1.00	2.143	1.918
5.5	1.00	2.333	2.630
5.6	1.00	2.535	2.954
5.7	1.00	2.745	3.301
5.8	1.00	2.957	3.661
5.9	1.00	3.166	4.022
6.0	1.00	3.366	4.374
6.1	1.00	3.492	4.587
6.2	1.00	3.722	5.006
6.3	1.00	3.871	4.164
6.4	1.00	4.000	4.341
6.5	1.00	4.107	5.690
6.6	1.00	4.193	5.838
6.7	1.00	4.259	5.945
6.8	1.00	4.306	6.013
6.9	1.00	4.334	6.042
7.0	1.00	4.343	6.031
7.1	1.00	4.255	5.829
7.2	1.00	4.308	5.889
7.3	1.00	4.262	4.528
7.4	1.00	4.196	4.386
7.5	1.00	4.108	5.346
7.6	1.00	3.996	5.069
7.7	1.00	3.860	4.744
7.8	1.00	3.698	4.373
7.9	1.00	3.510	3.962
8.0	1.00	3.298	3.522
8.1	1.00	3.006	2.978
8.2	1.00	2.811	2.606
8.3	1.00	2.546	1.702
8.4	1.00	2.276	1.378
8.5	1.00	2.008	1.383
8.6	1.00	1.748	1.067
8.7	1.00	1.503	0.805
8.8	1.00	1.278	0.595
8.9	1.00	1.075	0.432
9.0	1.00	0.896	0.310
9.1	1.00	0.727	0.208
9.2	1.00	0.608	0.154
9.3	1.00	0.496	0.085
9.4	1.00	0.403	0.060
9.5	1.00	0.326	0.053
9.6	1.00	0.262	0.037
9.7	1.00	0.211	0.026
9.8	1.00	0.169	0.019
9.9	1.00	0.135	0.014

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 56 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.980	0.990
3.1	0.980	0.990	1.000
3.2	0.990	0.990	1.010
3.3	0.990	1.000	1.010
3.4	0.990	1.010	1.020
3.5	0.994	1.018	1.031
3.6	0.995	1.027	1.042
3.7	1.00	1.038	1.054
3.8	1.00	1.051	1.070
3.9	1.00	0.848	0.864
4.0	1.00	1.080	1.110
4.1	1.00	1.107	1.142
4.2	1.00	1.135	1.178
4.3	1.00	1.170	1.224
4.4	1.00	1.213	1.281
4.5	1.00	1.266	1.352
4.6	1.00	1.332	1.441
4.7	1.00	1.413	1.551
4.8	1.00	1.512	1.687
4.9	1.00	1.322	1.479
5.0	1.00	1.780	2.060
5.1	1.00	1.950	2.306
5.2	1.00	2.153	2.602
5.3	1.00	2.390	2.953
5.4	1.00	2.660	3.360
5.5	1.00	2.964	3.824
5.6	1.00	3.297	4.342
5.7	1.00	3.655	4.906
5.8	1.00	4.029	5.502
5.9	1.00	3.915	5.349
6.0	1.00	4.788	6.725
6.1	1.00	5.151	7.314
6.2	1.00	5.490	7.870
6.3	1.00	5.797	8.362
6.4	1.00	6.067	8.793
6.5	1.00	6.296	9.150
6.6	1.00	6.481	9.429
6.7	1.00	6.623	9.627
6.8	1.00	6.722	9.741
6.9	1.00	6.697	9.706
7.0	1.00	6.790	9.716
7.1	1.00	6.760	9.574
7.2	1.00	6.686	9.344
7.3	1.00	6.568	9.023
7.4	1.00	6.403	8.613
7.5	1.00	6.192	8.115
7.6	1.00	5.933	7.536
7.7	1.00	5.629	6.887
7.8	1.00	5.281	6.184
7.9	1.00	5.277	6.179
8.0	1.00	4.483	4.707
8.1	1.00	4.050	3.985
8.2	1.00	3.610	3.308
8.3	1.00	3.175	2.695
8.4	1.00	2.756	2.159
8.5	1.00	2.364	1.705
8.6	1.00	2.004	1.331
8.7	1.00	1.682	1.030
8.8	1.00	1.399	0.792
8.9	1.00	1.398	0.792
9.0	1.00	0.946	0.465
9.1	1.00	0.771	0.357
9.2	1.00	0.625	0.274
9.3	1.00	0.505	0.211
9.4	1.00	0.407	0.164
9.5	1.00	0.327	0.127
9.6	1.00	0.262	0.099
9.7	1.00	0.209	0.077
9.8	1.00	0.167	0.061
9.9	1.00	0.167	0.061

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 57 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.990
3.1	0.980	0.980	0.990
3.2	0.990	0.990	1.000
3.3	0.990	1.000	1.000
3.4	0.990	1.000	1.010
3.5	0.994	1.008	1.011
3.6	0.995	1.015	1.017
3.7	1.00	1.022	1.023
3.8	1.00	1.031	1.031
3.9	1.00	1.041	1.040
4.0	1.00	1.050	1.050
4.1	1.00	1.069	1.066
4.2	1.00	1.088	1.084
4.3	1.00	1.110	1.107
4.4	1.00	1.139	1.135
4.5	1.00	1.174	1.171
4.6	1.00	1.217	1.217
4.7	1.00	1.270	1.274
4.8	1.00	1.334	1.347
4.9	1.00	1.413	1.437
5.0	1.00	1.510	1.550
5.1	1.00	1.620	1.690
5.2	1.00	1.753	1.860
5.3	1.00	1.908	2.065
5.4	1.00	2.085	2.307
5.5	1.00	2.283	2.587
5.6	1.00	2.501	2.902
5.7	1.00	2.734	3.249
5.8	1.00	2.979	3.619
5.9	1.00	3.228	4.001
6.0	1.00	3.474	4.384
6.1	1.00	3.711	4.756
6.2	1.00	3.930	5.100
6.3	1.00	4.131	5.418
6.4	1.00	4.307	5.690
6.5	1.00	4.454	5.916
6.6	1.00	4.574	6.091
6.7	1.00	4.664	6.213
6.8	1.00	4.726	6.282
6.9	1.00	4.758	6.295
7.0	1.00	4.762	6.253
7.1	1.00	4.737	6.154
7.2	1.00	4.682	5.996
7.3	1.00	4.596	5.780
7.4	1.00	4.479	5.504
7.5	1.00	4.330	5.171
7.6	1.00	4.148	4.785
7.7	1.00	3.934	4.354
7.8	1.00	3.691	3.889
7.9	1.00	3.422	3.404
8.0	1.00	3.132	2.918
8.1	1.00	2.829	2.448
8.2	1.00	2.522	2.010
8.3	1.00	2.218	1.616
8.4	1.00	1.925	1.276
8.5	1.00	1.651	0.990
8.6	1.00	1.400	0.759
8.7	1.00	1.175	0.575
8.8	1.00	0.977	0.433
8.9	1.00	0.806	0.325
9.0	1.00	0.661	0.243
9.1	1.00	0.538	0.182
9.2	1.00	0.437	0.137
9.3	1.00	0.353	0.104
9.4	1.00	0.284	0.079
9.5	1.00	0.228	0.060
9.6	1.00	0.183	0.046
9.7	1.00	0.146	0.036
9.8	1.00	0.117	0.028
9.9	1.00	0.093	0.022

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 58 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.980
3.1	0.980	0.980	0.990
3.2	0.990	0.990	0.990
3.3	0.990	0.990	0.990
3.4	0.990	1.000	1.000
3.5	0.994	1.002	0.999
3.6	0.995	1.007	1.002
3.7	1.00	1.013	1.004
3.8	1.00	1.019	1.007
3.9	1.00	1.027	1.011
4.0	1.00	1.040	1.010
4.1	1.00	1.046	1.020
4.2	1.00	1.058	1.026
4.3	1.00	1.074	1.035
4.4	1.00	1.093	1.046
4.5	1.00	1.117	1.060
4.6	1.00	1.146	1.079
4.7	1.00	1.182	1.104
4.8	1.00	1.225	1.137
4.9	1.00	1.278	1.181
5.0	1.00	1.340	1.240
5.1	1.00	1.418	1.311
5.2	1.00	1.507	1.404
5.3	1.00	1.612	1.519
5.4	1.00	1.731	1.659
5.5	1.00	1.864	1.825
5.6	1.00	2.011	2.016
5.7	1.00	2.168	2.229
5.8	1.00	2.332	2.460
5.9	1.00	2.500	2.701
6.0	1.00	2.665	2.944
6.1	1.00	2.824	3.181
6.2	1.00	2.970	3.400
6.3	1.00	3.106	3.606
6.4	1.00	3.223	3.781
6.5	1.00	3.321	3.925
6.6	1.00	3.400	4.036
6.7	1.00	3.459	4.112
6.8	1.00	3.497	4.153
6.9	1.00	3.516	4.156
7.0	1.00	3.514	4.122
7.1	1.00	3.492	4.049
7.2	1.00	3.448	3.936
7.3	1.00	3.383	3.784
7.4	1.00	3.295	3.591
7.5	1.00	3.184	3.360
7.6	1.00	3.049	3.093
7.7	1.00	2.892	2.795
7.8	1.00	2.712	2.477
7.9	1.00	2.514	2.147
8.0	1.00	2.301	1.817
8.1	1.00	2.078	1.502
8.2	1.00	1.852	1.210
8.3	1.00	1.629	0.952
8.4	1.00	1.414	0.732
8.5	1.00	1.212	0.551
8.6	1.00	1.028	0.407
8.7	1.00	0.863	0.295
8.8	1.00	0.717	0.212
8.9	1.00	0.592	0.151
9.0	1.00	0.485	0.106
9.1	1.00	0.395	0.075
9.2	1.00	0.321	0.053
9.3	1.00	0.259	0.037
9.4	1.00	0.208	0.027
9.5	1.00	0.167	0.019
9.6	1.00	0.134	0.014
9.7	1.00	0.107	0.010
9.8	1.00	0.086	0.007
9.9	1.00	0.068	0.006

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 59 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.980	1.000
3.1	0.980	0.990	1.010
3.2	0.990	1.000	1.020
3.3	0.990	1.010	1.030
3.4	0.990	1.020	1.040
3.5	0.994	1.036	1.057
3.6	0.995	1.050	1.074
3.7	1.00	1.066	1.094
3.8	1.00	1.086	1.120
3.9	1.00	1.110	1.152
4.0	1.00	1.140	1.190
4.1	1.00	1.176	1.241
4.2	1.00	1.222	1.303
4.3	1.00	1.277	1.380
4.4	1.00	1.347	1.477
4.5	1.00	1.432	1.598
4.6	1.00	1.536	1.748
4.7	1.00	1.663	1.934
4.8	1.00	1.816	2.162
4.9	1.00	2.000	2.442
5.0	1.00	2.220	2.780
5.1	1.00	2.474	3.185
5.2	1.00	2.769	3.662
5.3	1.00	3.103	4.213
5.4	1.00	3.473	4.837
5.5	1.00	3.876	5.527
5.6	1.00	4.303	6.269
5.7	1.00	4.745	7.047
5.8	1.00	5.189	7.839
5.9	1.00	5.624	8.620
6.0	1.00	6.038	9.368
6.1	1.00	6.422	10.064
6.2	1.00	6.770	10.690
6.3	1.00	7.072	11.240
6.4	1.00	7.332	11.704
6.5	1.00	7.546	12.081
6.6	1.00	7.718	12.370
6.7	1.00	7.847	12.573
6.8	1.00	7.936	12.692
6.9	1.00	7.986	12.726
7.0	1.00	7.998	12.677
7.1	1.00	7.972	12.543
7.2	1.00	7.907	12.319
7.3	1.00	7.803	12.004
7.4	1.00	7.656	11.591
7.5	1.00	7.464	11.080
7.6	1.00	7.226	10.468
7.7	1.00	6.938	9.760
7.8	1.00	6.601	8.964
7.9	1.00	6.217	8.097
8.0	1.00	5.790	7.182
8.1	1.00	5.327	6.247
8.2	1.00	4.839	5.326
8.3	1.00	4.338	4.450
8.4	1.00	3.837	3.645
8.5	1.00	3.349	2.932
8.6	1.00	2.888	2.321
8.7	1.00	2.460	1.813
8.8	1.00	2.074	1.401
8.9	1.00	1.732	1.074
9.0	1.00	1.434	0.820
9.1	1.00	1.178	0.625
9.2	1.00	0.962	0.477
9.3	1.00	0.782	0.364
9.4	1.00	0.633	0.279
9.5	1.00	0.510	0.214
9.6	1.00	0.410	0.166
9.7	1.00	0.329	0.128
9.8	1.00	0.263	0.100
9.9	1.00	0.211	0.078

Notes
Kow = n-octanol-water partition coefficient
Km = metabolic transformation rate constant
$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow
C = Celsius

Table 60 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.980	0.990
3.1	0.980	0.990	1.000
3.2	0.990	0.990	1.000
3.3	0.990	1.000	1.010
3.4	0.990	1.010	1.020
3.5	0.994	1.020	1.025
3.6	0.995	1.030	1.034
3.7	1.00	1.042	1.045
3.8	1.00	1.055	1.058
3.9	1.00	1.071	1.074
4.0	1.00	1.090	1.090
4.1	1.00	1.115	1.120
4.2	1.00	1.145	1.152
4.3	1.00	1.182	1.193
4.4	1.00	1.228	1.245
4.5	1.00	1.284	1.310
4.6	1.00	1.353	1.392
4.7	1.00	1.437	1.496
4.8	1.00	1.538	1.626
4.9	1.00	1.659	1.787
5.0	1.00	1.800	1.960
5.1	1.00	1.972	2.228
5.2	1.00	2.166	2.516
5.3	1.00	2.386	2.854
5.4	1.00	2.631	3.240
5.5	1.00	2.896	3.671
5.6	1.00	3.178	4.139
5.7	1.00	3.469	4.632
5.8	1.00	3.761	5.137
5.9	1.00	4.048	5.636
6.0	1.00	4.320	5.552
6.1	1.00	4.573	6.563
6.2	1.00	4.800	6.970
6.3	1.00	5.001	7.321
6.4	1.00	5.171	7.619
6.5	1.00	5.312	7.861
6.6	1.00	5.423	8.047
6.7	1.00	5.506	8.175
6.8	1.00	5.563	8.249
6.9	1.00	5.593	8.267
7.0	1.00	5.598	7.013
7.1	1.00	5.577	8.136
7.2	1.00	5.529	7.983
7.3	1.00	5.454	7.769
7.4	1.00	5.350	7.491
7.5	1.00	5.215	7.146
7.6	1.00	5.048	6.736
7.7	1.00	4.846	6.262
7.8	1.00	4.610	5.730
7.9	1.00	4.342	5.153
8.0	1.00	4.043	3.543
8.1	1.00	3.720	3.928
8.2	1.00	3.379	3.322
8.3	1.00	3.029	2.748
8.4	1.00	2.679	2.226
8.5	1.00	2.338	1.767
8.6	1.00	2.016	1.377
8.7	1.00	1.718	1.057
8.8	1.00	1.448	0.801
8.9	1.00	1.209	0.602
9.0	1.00	1.001	0.366
9.1	1.00	0.823	0.335
9.2	1.00	0.672	0.249
9.3	1.00	0.546	0.186
9.4	1.00	0.442	0.140
9.5	1.00	0.356	0.105
9.6	1.00	0.286	0.080
9.7	1.00	0.230	0.061
9.8	1.00	0.184	0.047
9.9	1.00	0.147	0.036

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 61 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.001)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.980
3.1	0.980	0.980	0.990
3.2	0.990	0.990	0.990
3.3	0.990	1.000	0.990
3.4	0.990	1.000	1.000
3.5	0.994	1.011	1.005
3.6	0.995	1.018	1.009
3.7	1.00	1.026	1.014
3.8	1.00	1.036	1.020
3.9	1.00	1.047	1.026
4.0	1.00	1.060	1.030
4.1	1.00	1.076	1.042
4.2	1.00	1.098	1.060
4.3	1.00	1.124	1.034
4.4	1.00	1.155	1.047
4.5	1.00	1.193	1.132
4.6	1.00	1.240	1.173
4.7	1.00	1.298	1.226
4.8	1.00	1.367	1.295
4.9	1.00	1.450	1.384
5.0	1.00	1.550	1.500
5.1	1.00	1.647	1.608
5.2	1.00	1.795	1.811
5.3	1.00	1.945	1.677
5.4	1.00	2.112	1.855
5.5	1.00	2.293	2.529
5.6	1.00	2.485	2.828
5.7	1.00	2.683	3.146
5.8	1.00	2.883	3.474
5.9	1.00	3.078	3.800
6.0	1.00	3.264	4.115
6.1	1.00	3.377	4.298
6.2	1.00	3.590	4.680
6.3	1.00	3.726	3.877
6.4	1.00	3.841	4.029
6.5	1.00	3.936	5.265
6.6	1.00	4.011	5.386
6.7	1.00	4.066	5.469
6.8	1.00	4.103	5.515
6.9	1.00	4.121	5.523
7.0	1.00	4.121	5.493
7.1	1.00	4.027	5.284
7.2	1.00	4.066	5.315
7.3	1.00	4.009	4.063
7.4	1.00	3.931	3.909
7.5	1.00	3.831	4.726
7.6	1.00	3.707	4.439
7.7	1.00	3.559	4.109
7.8	1.00	3.385	3.740
7.9	1.00	3.187	3.341
8.0	1.00	2.968	2.923
8.1	1.00	2.680	2.427
8.2	1.00	2.480	2.088
8.3	1.00	2.223	1.339
8.4	1.00	1.966	1.064
8.5	1.00	1.716	1.049
8.6	1.00	1.480	0.796
8.7	1.00	1.261	0.592
8.8	1.00	1.063	0.432
8.9	1.00	0.887	0.311
9.0	1.00	0.734	0.221
9.1	1.00	0.592	0.147
9.2	1.00	0.493	0.110
9.3	1.00	0.401	0.061
9.4	1.00	0.324	0.042
9.5	1.00	0.261	0.038
9.6	1.00	0.210	0.027
9.7	1.00	0.169	0.019
9.8	1.00	0.135	0.014
9.9	1.00	0.108	0.010

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 62 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.980	0.990
3.1	0.980	0.980	1.000
3.2	0.990	0.990	1.000
3.3	0.990	1.000	1.010
3.4	0.990	1.010	1.020
3.5	0.994	1.016	1.024
3.6	0.995	1.024	1.032
3.7	1.00	1.034	1.043
3.8	1.00	1.046	1.055
3.9	1.00	0.844	0.852
4.0	1.00	1.080	1.090
4.1	1.00	1.097	1.112
4.2	1.00	1.123	1.141
4.3	1.00	1.154	1.176
4.4	1.00	1.192	1.220
4.5	1.00	1.240	1.273
4.6	1.00	1.297	1.339
4.7	1.00	1.368	1.419
4.8	1.00	1.452	1.516
4.9	1.00	1.269	1.329
5.0	1.00	1.670	1.770
5.1	1.00	1.811	1.932
5.2	1.00	1.969	2.119
5.3	1.00	2.148	2.329
5.4	1.00	2.344	2.563
5.5	1.00	2.556	2.815
5.6	1.00	2.778	3.081
5.7	1.00	3.004	3.353
5.8	1.00	3.229	3.623
5.9	1.00	3.137	3.522
6.0	1.00	3.647	4.125
6.1	1.00	3.830	4.341
6.2	1.00	3.990	4.530
6.3	1.00	4.125	4.680
6.4	1.00	4.233	4.796
6.5	1.00	4.313	4.873
6.6	1.00	4.366	4.910
6.7	1.00	4.391	4.907
6.8	1.00	4.388	4.862
6.9	1.00	4.372	4.845
7.0	1.00	4.296	4.645
7.1	1.00	4.206	4.471
7.2	1.00	4.085	4.253
7.3	1.00	3.934	3.994
7.4	1.00	3.752	3.696
7.5	1.00	3.540	3.367
7.6	1.00	3.303	3.014
7.7	1.00	3.043	2.651
7.8	1.00	2.768	2.288
7.9	1.00	2.766	2.286
8.0	1.00	2.199	1.615
8.1	1.00	1.921	1.323
8.2	1.00	1.658	1.068
8.3	1.00	1.413	0.853
8.4	1.00	1.192	0.675
8.5	1.00	0.996	0.530
8.6	1.00	0.825	0.415
8.7	1.00	0.678	0.324
8.8	1.00	0.554	0.253
8.9	1.00	0.554	0.253
9.0	1.00	0.364	0.154
9.1	1.00	0.294	0.121
9.2	1.00	0.236	0.095
9.3	1.00	0.190	0.074
9.4	1.00	0.152	0.058
9.5	1.00	0.121	0.046
9.6	1.00	0.097	0.036
9.7	1.00	0.077	0.029
9.8	1.00	0.062	0.023
9.9	1.00	0.061	0.023

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 63 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.980
3.1	0.980	0.980	0.990
3.2	0.990	0.990	0.990
3.3	0.990	0.990	1.000
3.4	0.990	1.000	1.000
3.5	0.994	1.006	1.004
3.6	0.995	1.012	1.008
3.7	1.00	1.019	1.012
3.8	1.00	1.027	1.017
3.9	1.00	1.036	1.023
4.0	1.00	1.050	1.030
4.1	1.00	1.060	1.039
4.2	1.00	1.076	1.050
4.3	1.00	1.095	1.063
4.4	1.00	1.119	1.081
4.5	1.00	1.149	1.103
4.6	1.00	1.185	1.131
4.7	1.00	1.229	1.166
4.8	1.00	1.281	1.210
4.9	1.00	1.344	1.264
5.0	1.00	1.420	1.330
5.1	1.00	1.505	1.411
5.2	1.00	1.604	1.507
5.3	1.00	1.715	1.618
5.4	1.00	1.837	1.744
5.5	1.00	1.969	1.883
5.6	1.00	2.107	2.031
5.7	1.00	2.247	2.185
5.8	1.00	2.387	2.339
5.9	1.00	2.521	2.489
6.0	1.00	2.646	2.629
6.1	1.00	2.759	2.754
6.2	1.00	2.860	2.860
6.3	1.00	2.940	2.950
6.4	1.00	3.005	3.015
6.5	1.00	3.052	3.056
6.6	1.00	3.081	3.074
6.7	1.00	3.092	3.065
6.8	1.00	3.085	3.031
6.9	1.00	3.058	2.970
7.0	1.00	3.013	2.882
7.1	1.00	2.947	2.766
7.2	1.00	2.861	2.622
7.3	1.00	2.753	2.452
7.4	1.00	2.625	2.257
7.5	1.00	2.476	2.044
7.6	1.00	2.309	1.817
7.7	1.00	2.127	1.584
7.8	1.00	1.934	1.353
7.9	1.00	1.736	1.133
8.0	1.00	1.536	0.931
8.1	1.00	1.342	0.751
8.2	1.00	1.158	0.596
8.3	1.00	0.987	0.467
8.4	1.00	0.833	0.362
8.5	1.00	0.695	0.279
8.6	1.00	0.576	0.214
8.7	1.00	0.474	0.163
8.8	1.00	0.387	0.125
8.9	1.00	0.314	0.096
9.0	1.00	0.254	0.074
9.1	1.00	0.205	0.057
9.2	1.00	0.165	0.044
9.3	1.00	0.132	0.034
9.4	1.00	0.106	0.027
9.5	1.00	0.085	0.021
9.6	1.00	0.068	0.016
9.7	1.00	0.054	0.013
9.8	1.00	0.043	0.010
9.9	1.00	0.034	0.008

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 64 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.980
3.1	0.980	0.980	0.980
3.2	0.990	0.980	0.990
3.3	0.990	0.990	0.990
3.4	0.990	0.990	0.990
3.5	0.994	1.000	0.992
3.6	0.995	1.004	0.993
3.7	1.00	1.009	0.993
3.8	1.00	1.015	0.994
3.9	1.00	1.021	0.994
4.0	1.00	1.030	0.990
4.1	1.00	1.036	0.995
4.2	1.00	1.047	0.994
4.3	1.00	1.059	0.994
4.4	1.00	1.074	0.995
4.5	1.00	1.093	0.998
4.6	1.00	1.116	1.002
4.7	1.00	1.143	1.009
4.8	1.00	1.176	1.021
4.9	1.00	1.216	1.037
5.0	1.00	1.260	1.060
5.1	1.00	1.317	1.104
5.2	1.00	1.379	1.130
5.3	1.00	1.448	1.180
5.4	1.00	1.525	1.240
5.5	1.00	1.608	1.309
5.6	1.00	1.694	1.385
5.7	1.00	1.782	1.466
5.8	1.00	1.869	1.550
5.9	1.00	1.953	1.631
6.0	1.00	2.030	1.708
6.1	1.00	2.100	1.834
6.2	1.00	2.160	1.840
6.3	1.00	2.210	1.885
6.4	1.00	2.249	1.919
6.5	1.00	2.275	1.939
6.6	1.00	2.290	1.943
6.7	1.00	2.293	1.932
6.8	1.00	2.283	1.905
6.9	1.00	2.260	1.860
7.0	1.00	2.223	1.797
7.1	1.00	2.173	1.788
7.2	1.00	2.107	1.618
7.3	1.00	2.027	1.503
7.4	1.00	1.931	1.372
7.5	1.00	1.821	1.230
7.6	1.00	1.698	1.080
7.7	1.00	1.563	0.927
7.8	1.00	1.421	0.778
7.9	1.00	1.275	0.637
8.0	1.00	1.129	0.510
8.1	1.00	0.986	0.423
8.2	1.00	0.850	0.305
8.3	1.00	0.725	0.229
8.4	1.00	0.611	0.170
8.5	1.00	0.511	0.124
8.6	1.00	0.423	0.090
8.7	1.00	0.348	0.065
8.8	1.00	0.284	0.046
8.9	1.00	0.231	0.033
9.0	1.00	0.187	0.024
9.1	1.00	0.151	0.019
9.2	1.00	0.121	0.013
9.3	1.00	0.097	0.009
9.4	1.00	0.078	0.007
9.5	1.00	0.062	0.005
9.6	1.00	0.050	0.004
9.7	1.00	0.040	0.003
9.8	1.00	0.032	0.002
9.9	1.00	0.025	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 65 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.980	1.000
3.1	0.980	0.990	1.010
3.2	0.990	1.000	1.020
3.3	0.990	1.010	1.030
3.4	0.990	1.020	1.040
3.5	0.994	1.034	1.049
3.6	0.995	1.047	1.063
3.7	1.00	1.062	1.081
3.8	1.00	1.081	1.104
3.9	1.00	1.103	1.131
4.0	1.00	1.130	1.160
4.1	1.00	1.165	1.207
4.2	1.00	1.207	1.259
4.3	1.00	1.259	1.323
4.4	1.00	1.322	1.403
4.5	1.00	1.399	1.501
4.6	1.00	1.493	1.621
4.7	1.00	1.606	1.766
4.8	1.00	1.741	1.941
4.9	1.00	1.899	2.149
5.0	1.00	2.080	2.390
5.1	1.00	2.294	2.677
5.2	1.00	2.530	2.998
5.3	1.00	2.789	3.355
5.4	1.00	3.068	3.741
5.5	1.00	3.359	4.149
5.6	1.00	3.656	4.567
5.7	1.00	3.950	4.984
5.8	1.00	4.233	5.387
5.9	1.00	4.498	5.764
6.0	1.00	4.739	6.107
6.1	1.00	4.952	6.407
6.2	1.00	5.140	6.660
6.3	1.00	5.286	6.865
6.4	1.00	5.405	7.018
6.5	1.00	5.493	7.121
6.6	1.00	5.549	7.172
6.7	1.00	5.576	7.172
6.8	1.00	5.573	7.120
6.9	1.00	5.540	7.014
7.0	1.00	5.476	6.853
7.1	1.00	5.379	6.636
7.2	1.00	5.249	6.359
7.3	1.00	5.084	6.025
7.4	1.00	4.883	5.634
7.5	1.00	4.647	5.192
7.6	1.00	4.376	4.708
7.7	1.00	4.074	4.196
7.8	1.00	3.746	3.670
7.9	1.00	3.401	3.150
8.0	1.00	3.047	2.653
8.1	1.00	2.693	2.193
8.2	1.00	2.350	1.784
8.3	1.00	2.024	1.429
8.4	1.00	1.724	1.131
8.5	1.00	1.452	0.887
8.6	1.00	1.212	0.691
8.7	1.00	1.003	0.536
8.8	1.00	0.824	0.415
8.9	1.00	0.673	0.321
9.0	1.00	0.547	0.249
9.1	1.00	0.442	0.193
9.2	1.00	0.356	0.151
9.3	1.00	0.287	0.117
9.4	1.00	0.230	0.092
9.5	1.00	0.184	0.072
9.6	1.00	0.147	0.057
9.7	1.00	0.117	0.045
9.8	1.00	0.094	0.035
9.9	1.00	0.075	0.028

Notes
Kow = n-octanol-water partition coefficient
Km = metabolic transformation rate constant
$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow
C = Celsius

Table 66 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.980	0.990
3.1	0.980	0.990	0.990
3.2	0.990	0.990	1.000
3.3	0.990	1.000	1.010
3.4	0.990	1.010	1.010
3.5	0.994	1.018	1.017
3.6	0.995	1.027	1.024
3.7	1.00	1.038	1.032
3.8	1.00	1.050	1.042
3.9	1.00	1.065	1.055
4.0	1.00	1.080	1.070
4.1	1.00	1.105	1.089
4.2	1.00	1.132	1.113
4.3	1.00	1.165	1.144
4.4	1.00	1.206	1.182
4.5	1.00	1.255	1.230
4.6	1.00	1.315	1.290
4.7	1.00	1.388	1.364
4.8	1.00	1.474	1.457
4.9	1.00	1.575	1.569
5.0	1.00	1.690	1.700
5.1	1.00	1.828	1.863
5.2	1.00	1.979	2.047
5.3	1.00	2.145	2.254
5.4	1.00	2.323	2.482
5.5	1.00	2.510	2.724
5.6	1.00	2.699	2.976
5.7	1.00	2.887	3.228
5.8	1.00	3.068	3.473
5.9	1.00	3.237	3.704
6.0	1.00	3.391	3.913
6.1	1.00	3.527	4.097
6.2	1.00	3.640	4.250
6.3	1.00	3.738	4.377
6.4	1.00	3.812	4.469
6.5	1.00	3.866	4.529
6.6	1.00	3.900	4.557
6.7	1.00	3.913	4.552
6.8	1.00	3.907	4.513
6.9	1.00	3.880	4.440
7.0	1.00	3.833	4.331
7.1	1.00	3.763	4.184
7.2	1.00	3.671	4.000
7.3	1.00	3.554	3.778
7.4	1.00	3.413	3.520
7.5	1.00	3.247	3.229
7.6	1.00	3.057	2.912
7.7	1.00	2.845	2.578
7.8	1.00	2.617	2.237
7.9	1.00	2.375	1.902
8.0	1.00	2.128	1.583
8.1	1.00	1.881	1.292
8.2	1.00	1.641	1.035
8.3	1.00	1.413	0.815
8.4	1.00	1.203	0.633
8.5	1.00	1.014	0.487
8.6	1.00	0.846	0.371
8.7	1.00	0.700	0.282
8.8	1.00	0.575	0.214
8.9	1.00	0.470	0.162
9.0	1.00	0.382	0.123
9.1	1.00	0.309	0.094
9.2	1.00	0.249	0.072
9.3	1.00	0.200	0.055
9.4	1.00	0.160	0.043
9.5	1.00	0.128	0.033
9.6	1.00	0.103	0.026
9.7	1.00	0.082	0.020
9.8	1.00	0.065	0.016
9.9	1.00	0.052	0.012

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 67 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.01)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.970	0.980
3.1	0.980	0.980	0.990
3.2	0.990	0.990	0.990
3.3	0.990	1.000	0.990
3.4	0.990	1.000	0.990
3.5	0.994	1.008	0.998
3.6	0.995	1.015	1.000
3.7	1.00	1.022	1.002
3.8	1.00	1.031	1.005
3.9	1.00	1.041	1.008
4.0	1.00	1.050	1.010
4.1	1.00	1.066	1.013
4.2	1.00	1.086	1.024
4.3	1.00	1.107	0.992
4.4	1.00	1.134	0.994
4.5	1.00	1.167	1.063
4.6	1.00	1.206	1.086
4.7	1.00	1.253	1.117
4.8	1.00	1.310	1.158
4.9	1.00	1.376	1.212
5.0	1.00	1.450	1.280
5.1	1.00	1.527	1.336
5.2	1.00	1.640	1.461
5.3	1.00	1.749	1.316
5.4	1.00	1.865	1.408
5.5	1.00	1.987	1.848
5.6	1.00	2.111	1.997
5.7	1.00	2.234	2.148
5.8	1.00	2.351	2.296
5.9	1.00	2.462	2.436
6.0	1.00	2.562	2.564
6.1	1.00	2.604	2.603
6.2	1.00	2.720	2.770
6.3	1.00	2.785	2.250
6.4	1.00	2.832	2.291
6.5	1.00	2.865	2.935
6.6	1.00	2.884	2.948
6.7	1.00	2.890	2.939
6.8	1.00	2.882	2.909
6.9	1.00	2.859	2.855
7.0	1.00	2.822	2.778
7.1	1.00	2.718	2.598
7.2	1.00	2.699	2.548
7.3	1.00	2.612	1.886
7.4	1.00	2.508	1.747
7.5	1.00	2.385	2.021
7.6	1.00	2.245	1.807
7.7	1.00	2.090	1.582
7.8	1.00	1.921	1.355
7.9	1.00	1.744	1.133
8.0	1.00	1.562	0.925
8.1	1.00	1.355	0.709
8.2	1.00	1.204	0.574
8.3	1.00	1.037	0.344
8.4	1.00	0.883	0.257
8.5	1.00	0.744	0.240
8.6	1.00	0.621	0.174
8.7	1.00	0.514	0.125
8.8	1.00	0.422	0.090
8.9	1.00	0.345	0.064
9.0	1.00	0.280	0.045
9.1	1.00	0.222	0.029
9.2	1.00	0.183	0.023
9.3	1.00	0.147	0.013
9.4	1.00	0.118	0.010
9.5	1.00	0.094	0.009
9.6	1.00	0.075	0.007
9.7	1.00	0.060	0.005
9.8	1.00	0.048	0.004
9.9	1.00	0.038	0.003

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 68 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.968	0.968
3.1	0.984	0.975	0.969
3.2	0.987	0.981	0.968
3.3	0.990	0.985	0.966
3.4	0.992	0.989	0.962
3.5	0.994	0.993	0.957
3.6	0.995	0.996	0.950
3.7	1.00	0.998	0.941
3.8	1.00	1.001	0.930
3.9	1.00	0.807	0.751
4.0	1.00	1.006	0.902
4.1	1.00	1.009	0.886
4.2	1.00	1.012	0.867
4.3	1.00	1.015	0.847
4.4	1.00	1.019	0.827
4.5	1.00	1.023	0.805
4.6	1.00	1.028	0.784
4.7	1.00	1.033	0.764
4.8	1.00	1.039	0.744
4.9	1.00	0.908	0.653
5.0	1.00	1.051	0.710
5.1	1.00	1.057	0.696
5.2	1.00	1.062	0.684
5.3	1.00	1.067	0.673
5.4	1.00	1.072	0.664
5.5	1.00	1.076	0.656
5.6	1.00	1.079	0.649
5.7	1.00	1.080	0.643
5.8	1.00	1.081	0.637
5.9	1.00	1.050	0.619
6.0	1.00	1.078	0.625
6.1	1.00	1.075	0.619
6.2	1.00	1.069	0.612
6.3	1.00	1.062	0.604
6.4	1.00	1.052	0.595
6.5	1.00	1.040	0.585
6.6	1.00	1.024	0.572
6.7	1.00	1.005	0.557
6.8	1.00	0.981	0.539
6.9	1.00	0.977	0.537
7.0	1.00	0.919	0.495
7.1	1.00	0.880	0.467
7.2	1.00	0.835	0.437
7.3	1.00	0.785	0.403
7.4	1.00	0.730	0.368
7.5	1.00	0.670	0.330
7.6	1.00	0.608	0.293
7.7	1.00	0.544	0.256
7.8	1.00	0.481	0.221
7.9	1.00	0.480	0.220
8.0	1.00	0.361	0.158
8.1	1.00	0.307	0.131
8.2	1.00	0.259	0.108
8.3	1.00	0.216	0.089
8.4	1.00	0.179	0.072
8.5	1.00	0.147	0.058
8.6	1.00	0.120	0.047
8.7	1.00	0.097	0.038
8.8	1.00	0.079	0.030
8.9	1.00	0.079	0.030
9.0	1.00	0.051	0.019
9.1	1.00	0.041	0.015
9.2	1.00	0.033	0.012
9.3	1.00	0.026	0.010
9.4	1.00	0.021	0.008
9.5	1.00	0.017	0.006
9.6	1.00	0.013	0.005
9.7	1.00	0.011	0.004
9.8	1.00	0.008	0.003
9.9	1.00	0.008	0.003

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 69 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.964	0.961
3.1	0.984	0.971	0.961
3.2	0.987	0.976	0.958
3.3	0.990	0.979	0.954
3.4	0.992	0.981	0.947
3.5	0.994	0.983	0.938
3.6	0.995	0.984	0.927
3.7	1.00	0.983	0.913
3.8	1.00	0.982	0.896
3.9	1.00	0.980	0.876
4.0	1.00	0.978	0.853
4.1	1.00	0.974	0.827
4.2	1.00	0.969	0.798
4.3	1.00	0.963	0.766
4.4	1.00	0.957	0.732
4.5	1.00	0.948	0.696
4.6	1.00	0.939	0.660
4.7	1.00	0.928	0.624
4.8	1.00	0.917	0.589
4.9	1.00	0.904	0.556
5.0	1.00	0.891	0.525
5.1	1.00	0.878	0.496
5.2	1.00	0.865	0.471
5.3	1.00	0.852	0.448
5.4	1.00	0.840	0.428
5.5	1.00	0.829	0.411
5.6	1.00	0.818	0.396
5.7	1.00	0.808	0.383
5.8	1.00	0.799	0.372
5.9	1.00	0.791	0.363
6.0	1.00	0.782	0.354
6.1	1.00	0.774	0.346
6.2	1.00	0.766	0.339
6.3	1.00	0.757	0.331
6.4	1.00	0.747	0.324
6.5	1.00	0.736	0.316
6.6	1.00	0.723	0.307
6.7	1.00	0.707	0.297
6.8	1.00	0.690	0.286
6.9	1.00	0.669	0.274
7.0	1.00	0.645	0.260
7.1	1.00	0.617	0.244
7.2	1.00	0.585	0.226
7.3	1.00	0.550	0.207
7.4	1.00	0.511	0.187
7.5	1.00	0.469	0.167
7.6	1.00	0.425	0.146
7.7	1.00	0.380	0.127
7.8	1.00	0.336	0.108
7.9	1.00	0.293	0.091
8.0	1.00	0.252	0.075
8.1	1.00	0.215	0.062
8.2	1.00	0.181	0.051
8.3	1.00	0.151	0.041
8.4	1.00	0.125	0.033
8.5	1.00	0.102	0.027
8.6	1.00	0.084	0.021
8.7	1.00	0.068	0.017
8.8	1.00	0.055	0.014
8.9	1.00	0.044	0.011
9.0	1.00	0.036	0.009
9.1	1.00	0.029	0.007
9.2	1.00	0.023	0.005
9.3	1.00	0.018	0.004
9.4	1.00	0.015	0.003
9.5	1.00	0.012	0.003
9.6	1.00	0.009	0.002
9.7	1.00	0.007	0.002
9.8	1.00	0.006	0.001
9.9	1.00	0.005	0.001

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 70 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993;
$\Pi_{SOCW/Kow}$ = 2, Temperature = 8º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.962	0.957
3.1	0.984	0.968	0.956
3.2	0.987	0.972	0.952
3.3	0.990	0.975	0.946
3.4	0.992	0.977	0.938
3.5	0.994	0.977	0.927
3.6	0.995	0.976	0.913
3.7	1.00	0.974	0.896
3.8	1.00	0.971	0.876
3.9	1.00	0.966	0.851
4.0	1.00	0.960	0.823
4.1	1.00	0.953	0.791
4.2	1.00	0.943	0.755
4.3	1.00	0.932	0.716
4.4	1.00	0.918	0.673
4.5	1.00	0.902	0.629
4.6	1.00	0.884	0.584
4.7	1.00	0.864	0.538
4.8	1.00	0.842	0.493
4.9	1.00	0.818	0.451
5.0	1.00	0.793	0.410
5.1	1.00	0.768	0.373
5.2	1.00	0.744	0.340
5.3	1.00	0.720	0.310
5.4	1.00	0.697	0.283
5.5	1.00	0.677	0.260
5.6	1.00	0.658	0.240
5.7	1.00	0.641	0.224
5.8	1.00	0.626	0.209
5.9	1.00	0.612	0.197
6.0	1.00	0.600	0.187
6.1	1.00	0.589	0.178
6.2	1.00	0.579	0.170
6.3	1.00	0.569	0.163
6.4	1.00	0.559	0.157
6.5	1.00	0.548	0.150
6.6	1.00	0.537	0.144
6.7	1.00	0.525	0.138
6.8	1.00	0.510	0.131
6.9	1.00	0.494	0.123
7.0	1.00	0.476	0.115
7.1	1.00	0.455	0.106
7.2	1.00	0.431	0.097
7.3	1.00	0.404	0.087
7.4	1.00	0.376	0.077
7.5	1.00	0.345	0.066
7.6	1.00	0.312	0.056
7.7	1.00	0.280	0.047
7.8	1.00	0.247	0.039
7.9	1.00	0.215	0.031
8.0	1.00	0.185	0.025
8.1	1.00	0.158	0.019
8.2	1.00	0.133	0.015
8.3	1.00	0.111	0.012
8.4	1.00	0.092	0.009
8.5	1.00	0.075	0.007
8.6	1.00	0.061	0.005
8.7	1.00	0.050	0.004
8.8	1.00	0.040	0.003
8.9	1.00	0.033	0.002
9.0	1.00	0.026	0.002
9.1	1.00	0.021	0.002
9.2	1.00	0.017	0.001
9.3	1.00	0.013	0.001
9.4	1.00	0.011	0.001
9.5	1.00	0.009	0.001
9.6	1.00	0.007	0.000
9.7	1.00	0.005	0.000
9.8	1.00	0.004	0.000
9.9	1.00	0.003	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 71 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 23, Temperature = 16° C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.973	0.974
3.1	0.984	0.982	0.976
3.2	0.987	0.989	0.977
3.3	0.990	0.996	0.978
3.4	0.992	1.002	0.977
3.5	0.994	1.008	0.975
3.6	0.995	1.015	0.972
3.7	1.00	1.022	0.969
3.8	1.00	1.031	0.964
3.9	1.00	1.040	0.959
4.0	1.00	1.052	0.954
4.1	1.00	1.065	0.948
4.2	1.00	1.080	0.943
4.3	1.00	1.098	0.938
4.4	1.00	1.119	0.934
4.5	1.00	1.142	0.931
4.6	1.00	1.169	0.930
4.7	1.00	1.198	0.931
4.8	1.00	1.229	0.933
4.9	1.00	1.261	0.937
5.0	1.00	1.294	0.943
5.1	1.00	1.327	0.950
5.2	1.00	1.359	0.957
5.3	1.00	1.388	0.964
5.4	1.00	1.415	0.971
5.5	1.00	1.439	0.977
5.6	1.00	1.459	0.982
5.7	1.00	1.476	0.986
5.8	1.00	1.489	0.988
5.9	1.00	1.498	0.988
6.0	1.00	1.504	0.987
6.1	1.00	1.506	0.983
6.2	1.00	1.505	0.977
6.3	1.00	1.499	0.969
6.4	1.00	1.490	0.957
6.5	1.00	1.476	0.943
6.6	1.00	1.457	0.924
6.7	1.00	1.432	0.901
6.8	1.00	1.401	0.873
6.9	1.00	1.364	0.840
7.0	1.00	1.319	0.801
7.1	1.00	1.265	0.757
7.2	1.00	1.204	0.707
7.3	1.00	1.134	0.652
7.4	1.00	1.057	0.593
7.5	1.00	0.973	0.532
7.6	1.00	0.885	0.470
7.7	1.00	0.794	0.409
7.8	1.00	0.704	0.351
7.9	1.00	0.615	0.297
8.0	1.00	0.531	0.249
8.1	1.00	0.453	0.206
8.2	1.00	0.382	0.169
8.3	1.00	0.320	0.137
8.4	1.00	0.265	0.111
8.5	1.00	0.218	0.090
8.6	1.00	0.178	0.072
8.7	1.00	0.145	0.058
8.8	1.00	0.117	0.046
8.9	1.00	0.095	0.037
9.0	1.00	0.076	0.029
9.1	1.00	0.061	0.023
9.2	1.00	0.049	0.019
9.3	1.00	0.039	0.015
9.4	1.00	0.031	0.012
9.5	1.00	0.025	0.009
9.6	1.00	0.020	0.007
9.7	1.00	0.016	0.006
9.8	1.00	0.013	0.005
9.9	1.00	0.010	0.004

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 72 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 10, Temperature = 16° C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.968	0.964
3.1	0.984	0.975	0.963
3.2	0.987	0.981	0.962
3.3	0.990	0.986	0.958
3.4	0.992	0.989	0.953
3.5	0.994	0.993	0.945
3.6	0.995	0.996	0.936
3.7	1.00	0.999	0.925
3.8	1.00	1.001	0.911
3.9	1.00	1.004	0.895
4.0	1.00	1.007	0.879
4.1	1.00	1.009	0.856
4.2	1.00	1.013	0.833
4.3	1.00	1.016	0.809
4.4	1.00	1.020	0.785
4.5	1.00	1.025	0.760
4.6	1.00	1.030	0.736
4.7	1.00	1.035	0.712
4.8	1.00	1.040	0.691
4.9	1.00	1.046	0.671
5.0	1.00	1.052	0.729
5.1	1.00	1.058	0.638
5.2	1.00	1.063	0.625
5.3	1.00	1.068	0.614
5.4	1.00	1.072	0.604
5.5	1.00	1.075	0.596
5.6	1.00	1.078	0.589
5.7	1.00	1.079	0.582
5.8	1.00	1.079	0.576
5.9	1.00	1.078	0.571
6.0	1.00	1.076	0.921
6.1	1.00	1.073	0.559
6.2	1.00	1.067	0.552
6.3	1.00	1.060	0.544
6.4	1.00	1.051	0.535
6.5	1.00	1.039	0.525
6.6	1.00	1.024	0.512
6.7	1.00	1.005	0.498
6.8	1.00	0.982	0.480
6.9	1.00	0.955	0.460
7.0	1.00	0.923	0.852
7.1	1.00	0.885	0.410
7.2	1.00	0.842	0.380
7.3	1.00	0.793	0.348
7.4	1.00	0.738	0.314
7.5	1.00	0.680	0.279
7.6	1.00	0.618	0.244
7.7	1.00	0.555	0.210
7.8	1.00	0.491	0.178
7.9	1.00	0.430	0.148
8.0	1.00	0.371	0.257
8.1	1.00	0.316	0.100
8.2	1.00	0.267	0.081
8.3	1.00	0.223	0.065
8.4	1.00	0.185	0.052
8.5	1.00	0.152	0.041
8.6	1.00	0.124	0.033
8.7	1.00	0.101	0.026
8.8	1.00	0.082	0.021
8.9	1.00	0.066	0.016
9.0	1.00	0.053	0.020
9.1	1.00	0.043	0.010
9.2	1.00	0.034	0.008
9.3	1.00	0.027	0.007
9.4	1.00	0.022	0.005
9.5	1.00	0.017	0.004
9.6	1.00	0.014	0.003
9.7	1.00	0.011	0.003
9.8	1.00	0.009	0.002
9.9	1.00	0.007	0.002

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

Table 73 - Foodchain Multipliers for Warmwater Pelagic Foodweb Model (Gobas 1993; $\Pi_{SOCW/Kow}$ = 2, Temperature = 16º C, K_m = 0.1)

Log K_{ow}	Trophic Level 2	Trophic Level 3	Trophic Level 4
3.0	0.980	0.965	0.957
3.1	0.984	0.971	0.955
3.2	0.987	0.976	0.952
3.3	0.990	0.979	0.942
3.4	0.992	0.982	0.933
3.5	0.994	0.983	0.927
3.6	0.995	0.984	0.914
3.7	1.00	0.984	0.898
3.8	1.00	0.983	0.878
3.9	1.00	0.981	0.855
4.0	1.00	0.979	0.828
4.1	1.00	0.974	0.796
4.2	1.00	0.971	0.766
4.3	1.00	0.966	0.704
4.4	1.00	0.960	0.663
4.5	1.00	0.952	0.655
4.6	1.00	0.944	0.616
4.7	1.00	0.935	0.578
4.8	1.00	0.925	0.542
4.9	1.00	0.914	0.507
5.0	1.00	0.903	0.475
5.1	1.00	0.883	0.437
5.2	1.00	0.881	0.421
5.3	1.00	0.870	0.343
5.4	1.00	0.860	0.322
5.5	1.00	0.851	0.361
5.6	1.00	0.843	0.347
5.7	1.00	0.835	0.334
5.8	1.00	0.827	0.323
5.9	1.00	0.820	0.314
6.0	1.00	0.813	0.305
6.1	1.00	0.792	0.284
6.2	1.00	0.798	0.290
6.3	1.00	0.790	0.226
6.4	1.00	0.781	0.220
6.5	1.00	0.770	0.268
6.6	1.00	0.757	0.259
6.7	1.00	0.742	0.249
6.8	1.00	0.725	0.238
6.9	1.00	0.704	0.226
7.0	1.00	0.679	0.212
7.1	1.00	0.639	0.186
7.2	1.00	0.619	0.180
7.3	1.00	0.583	0.127
7.4	1.00	0.543	0.112
7.5	1.00	0.499	0.123
7.6	1.00	0.454	0.105
7.7	1.00	0.407	0.087
7.8	1.00	0.361	0.071
7.9	1.00	0.315	0.057
8.0	1.00	0.272	0.045
8.1	1.00	0.228	0.032
8.2	1.00	0.196	0.027
8.3	1.00	0.164	0.016
8.4	1.00	0.136	0.012
8.5	1.00	0.112	0.012
8.6	1.00	0.091	0.009
8.7	1.00	0.074	0.007
8.8	1.00	0.060	0.005
8.9	1.00	0.048	0.004
9.0	1.00	0.039	0.003
9.1	1.00	0.031	0.002
9.2	1.00	0.025	0.002
9.3	1.00	0.020	0.001
9.4	1.00	0.016	0.001
9.5	1.00	0.013	0.001
9.6	1.00	0.010	0.001
9.7	1.00	0.008	0.001
9.8	1.00	0.006	0.000
9.9	1.00	0.005	0.000

Notes

K_{ow} = n-octanol-water partition coefficient

K_m = metabolic transformation rate constant

$\Pi_{SOCW/Kow}$ = ratio of sediment-water concentration quotient and Kow

C = Celsius

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