SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

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ACRONYMS and ABBREVIATIONS

AALAC  Ambient Aquatic Life Advisory Concentrations
ACGIH  American Conference of Governmental Industrial Hygienists
ATSDR  Agency for Toxic Substances and Disease Registry
AWQC  Ambient Water Quality Criteria
BCF   Bioconcentration Factor
CAS RN Chemical Abstracts Survey Registration Number
CCC   Criteria Continuous Concentration
CERCLA Comprehensive Environmental Response, Compensation, and Liability Act
CFR   Code of Federal Regulations
CMC   Criteria Maximum Concentration
ED    Effective Dose
EPA   United States Environmental Protection Agency
EPI   Estimation Programs Interface
FDAAL Food and Drug Administration Action Levels
fs    Sorbent Content (fraction of clays plus organic carbon)
HEAST Health Effects Assessment Summary Tables
HEDR  Handbook of Environmental Degradation Rates
HLC   Henry’s Law Constant
HRS   Hazard Ranking System
HTF   Human Toxicity Factor
ICRP  International Commission on Radiological Protection
Int   Intermediate
IRIS  Integrated Risk Information System
IUR   Inhalation Unit Risk
Kd    Soil/Water Distribution Coefficient
Koc   Soil Organic/Carbon Partition Coefficient
LC    Lethal Concentration
LD    Lethal Dose
Log Kow Logarithm of the n-Octanol-Water Partition Coefficient
MCI   Molecular Connectivity Index
MCLs  Maximum Contaminant Levels
MCLGs Maximum Contaminant Level Goals
MRL  Minimal Risk Level
MW    Molecular Weight
NAAQS National Ambient Air Quality Standards
NESHAPs National Emission Standards for Hazardous Air Pollutants
NHL   Non-Hodgkin’s Lymphoma
NIOSH National Institute for Occupational Safety and Health
NJDEP New Jersey Department of Environmental Protection
NPL  National Priorities List
OEHHA California Environmental Protection Agency Office of Environmental Health Hazard Assessment
OSRTI Office of Superfund Remediation and Technology Innovation
PAH   Polyaromatic Hydrocarbons
PCB   Polychlorinated Biphenyls
PPRTV Provisional Peer Reviewed Toxicity Values
PRG   Preliminary Remediation Goals
RBA   Relative Bioavailability Adjustment
REL Reference Exposure Level
RfC Reference Concentration
RfD Reference Dose
RME Reasonable Maximum Exposure
RTECS Registry of Toxic Effects of Chemical Substances
RTI Research Triangle Institute
SC Screening Concentration
SCDM Superfund Chemical Data Matrix
SF Slope Factor (Cancer)
SPHEM Superfund Public Health Evaluation Manual
SRC Syracuse Research Corporation
STSC Superfund Health Risk Technical Support Center
TCDD 2,3,7,8-Tetrachlorodibenzo-p-dioxin
TCE trichloroethylene
TEF Toxicity Equivalence Factor
UMTRCA Uranium Mill Tailings Radiation Control Act
WOE Weight-of-Evidence
SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

[June 2014]

1.0 INTRODUCTION

The Superfund Chemical Data Matrix (SCDM) contains factor values and screening concentration benchmarks that can be used when applying the Hazard Ranking System (HRS; 40 CFR Part 300 Appendix A, 55 FR 51583) to evaluate potential National Priorities List (NPL) sites. The HRS assigns factor values for toxicity, gas migration potential, gas and ground water mobility, surface water persistence, and bioaccumulation potential. These assignments are based on the physical, chemical, ecological, toxicological, and radiological properties of hazardous substances present at a site. Hazardous substances, as defined for HRS purposes, include both hazardous substances referenced in the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) section 101(14), which are substances specifically listed under other federal laws and are known as “CERCLA hazardous substances,” and “pollutants or contaminants” as defined in CERCLA itself in section 101(33).

SCDM contains HRS factor values and benchmarks for those hazardous substances frequently found at sites that are evaluated using the HRS. SCDM also contains the physical, chemical, toxicological, and radiological input data used to calculate the factors and benchmarks. The input data presented in SCDM are taken directly from peer reviewed, generally accepted literature sources and databases and/or U.S. Environmental Protection Agency (EPA) developed literature sources and databases; or are calculated using procedures set forth by the EPA and in the HRS. Further HRS procedures are then applied to the input data to determine factor values and benchmarks, which include both risk-based screening concentrations and concentrations specified in regulatory limits for the hazardous substances.

This document explains the procedures used to provide chemical and physical properties, factor values and screening concentration benchmarks for substances listed in SCDM. The factor values and benchmarks supersede any previous values provided by SCDM, beginning January 2014. These new values and benchmarks reflect the EPA’s methodology for determining risk, as described in the EPA’s Risk Assessment Guidance for Superfund (RAGS) Volume 1: Human Health Evaluation Manual, Part F: Supplemental Guidance for Inhalation Risk Assessment and Part B: Development of Risk-based Preliminary Remediation Goals (EPA-540-R-070-002/OSWER 9285.7-82) and Soil Screening Guidance: Technical Background Document (EPA/540/R95/128).

Section 2.0 (Data Selection Methodology) of this document explains how data are selected and prioritized for use in assigning SCDM values. Section 3.0 (Calculation of Interim Values) describes how some values (e.g., half-lives, distribution coefficients, slope factors and water solubility for metals) are calculated using data and methodologies from published literature or regulatory guidance documents. Section 4.0 (Screening Concentration Benchmarks) describes how screening concentration benchmarks are calculated for air, water, soil and human food chain exposures. Section 5.0 (SCDM Data Reporting and Appendices) describes how SCDM data, HRS factor values, and screening concentration benchmarks are presented in the SCDM Appendices.

Data inputs, factor values and benchmarks are listed, by substance, in SCDM Appendix A. Appendices BI and BII contain tables presenting HRS factor values and benchmarks, organized by pathway. Appendix C contains a cross-reference index of substance name synonyms.
2.0 DATA SELECTION METHODOLOGY

This section describes the methodology used for collecting and selecting data to determine factor values and screening concentration benchmarks for the substances listed in SCDM. It also specifies data source reference hierarchies and how the hierarchies are applied for each data type.

Section 2.1 describes hazardous substance identification protocols and how they relate to special cases. Sections 2.2 through 2.9 specify the references used to obtain data and the methodologies used to extract the data and assign values. The criteria described in these sections were developed based on the type and quality of data available in the current SCDM references; they are not intended to apply to all data in general.

2.1 General Protocols for SCDM Data Collection

Compiling data for SCDM requires a determination of which data reasonably apply to each hazardous substance. In most cases, data are collected for each substance from the specific references identified in Sections 2.2 through 2.8. In some cases, however, data in the references cited are available only for a class or mixture of hazardous substances and not for the individual substances that are included in the class or that make up the mixture. In general, if any of these classes or mixtures is present at a hazardous waste site, it is assumed that the most toxic, most persistent, or most bioaccumulative component of the class or mixture is present. For these mixtures or classes, SCDM collects and uses those data resulting in the greatest HRS factor values as specified by the HRS (e.g., lowest Reference Dose [RfD], highest cancer slope factor [SF], longest half-life and greatest bioaccumulation factor) from the data provided in the references used. In other cases, data that are specific to individual substances are used or substituted as representative for a class of substances. These special cases are described in Sections 2.1.1 through 2.1.4 below.

2.1.1 Generic Values

SCDM contains generic values for the following classes of compounds:

- Chromium (III and VI oxidation states) – SCDM contains values for chromium III, chromium VI, and a “generic” total chromium value to be used only when the specific oxidation state is not known. SCDM assigns the oral RfD and reference concentration (RfC) from chromium VI to total chromium.

- Mercury (elemental and inorganic compounds) – SCDM contains data for elemental and inorganic species of mercury, and applies the data to a single listing of “mercury.” The oral RfD is for mercuric chloride, and the inhalation RfD is for elemental mercury vapor. The vapor pressure, Henry’s Law Constant and distribution coefficient are for elemental mercury. A geometric mean water solubility is based on the lowest solubility (mercurous chloride) and highest solubility (mercury perchlorate) found in the reference sources.

- Polychlorinated biphenyls (PCBs) – PCBs are represented as a single class of compounds, regardless of the PCB mixture or mixtures that may be identified at a site. For PCBs, toxicity in SCDM is based on Arochlor 1254, which results in the most environmentally conservative screening concentration benchmarks and bioaccumulation/human food chain-based factor values for this group of compounds. EPA’s most recent reference on PCB risk assessment is “EPA’s PCB Risk Assessment Review Guidance Document, Interim Draft,” 2000a.
• Endosulfans – SCDM contains data for endosulfan mixture and two endosulfan isomers (endosulfan I and endosulfan II). The RfD and distribution coefficient data are collected for endosulfan and applied to endosulfan mixture and its isomers. SCDM contains a vapor pressure and Henry’s Law constant for each isomer.

• Chlordane (alpha and gamma) – SCDM contains some data for the alpha and gamma isomers of chlordane, but most values represent a mixture of the two. When a reference does not specify whether chlordane data were derived from a specific isomer or isomer concentration, SCDM uses the generic values.

2.1.2 Use of Compound Classes to Assign Values for Individual Substances

SCDM assigns substance class data to the substances listed below. If no data can be found in the specified references for an individual substance, but data are available for the generic class to which the substance belongs, SCDM assigns the generic value to that substance. These substance classes contain relatively small sets of isomers, which are likely to occur as mixtures, and are well defined, in that the generic class typically refers to a mixture of all members of the class (e.g., o-, m-, p-xylene). Members of these classes are also expected to have similar chemical behavior.

• Polychlorinated dibenzo-dioxins and furans – SCDM contains cancer slope factor, inhalation unit risk (IUR) and RfD values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). When a slope factor, IUR and/or RfD are not available for similar dioxins and furans listed in SCDM, SCDM applies toxicity equivalence factors (TEFs) to determine the values for these substances. Substance-specific TEFs are obtained from EPA’s Recommended Toxicity Equivalence Factors (TEFs) for Human Health Risk Assessments of 2,3,7,8-Tetrachlorodibenzo-p-dioxin and Dioxin-Like Compounds (EPA/100/R 10/005), December 2010. All members of this class are assigned the weight of evidence (WOE) assigned to TCDD, which is currently B2.

• Polyaromatic hydrocarbons (PAHs) – SCDM contains cancer slope factor and IUR values for benzo(a)pyrene. When a slope factor and/or IUR are not available for similar PAHs listed in SCDM, SCDM applies TEFs to determine values for these substances. PAH-specific TEFs are obtained from EPA’s Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089), July 1993.

• Xylenes – Values are provided for o-xylene, m-xylene and p-xylene. If no data can be found in the specified references for the individual substances, but data are available for the generic class of xylenes, SCDM assigns the generic value to the individual substances. The class of xylenes is a relatively small set of isomers that are likely to occur as mixtures. The class also is well defined in that the generic class (e.g., xylenes) almost always refers to a mixture of all members of the class (o-, m-, and p-xylene). The expected similarity in chemical behavior for members of each class, as well as the likelihood that they will occur as mixtures, makes using data from mixtures reasonable.

• Dibutyltin compounds – SCDM assigns an RfD for dibutyltin dichloride using the following molecular weight conversion of the RfD assigned to dibutyltin: RfD (dibutyltin dichloride) = RfD (dibutyltin) x [molecular weight (dibutyltin dichloride) / molecular weight (dibutyltin)].

• Tributyltin compounds – SCDM assigns an RfD for tributyltin chloride using the following molecular weight conversion of the RfD assigned to tributyltin: RfD (tributyltin chloride) = RfD (tributyltin) x [molecular weight (tributyltin chloride) / molecular weight (tributyltin)].
2.1.3 Substitution Classes

In some cases, SCDM uses data from a parent substance class, for particular substances of that class. SCDM contains three major classes of data for which data substitution may be applied: (1) toxicity, (2) ground water mobility and (3) other. All toxicity data used to determine human- or eco-toxicity factor values can be substituted. Ground water mobility data substitutions include water solubility, geometric mean water solubility and soil/water distribution coefficient (Kd). Parent class data also may be used for hydrolysis, biodegradation, photolysis and volatilization half-lives, as well as bioconcentration factor (BCF) and logarithm of the n-octanol-water partition coefficient (Log Kow).

Currently in SCDM, two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for ground water mobility values with the elemental metal as the class parent. Radioactive isotopes may inherit data from the primary radioactive element. Substitute data are not applied to radioactive isotope decay chains.

2.1.4 Substances with Unique Value Selection

- Cadmium – For cadmium, the Integrated Risk Information System (IRIS) contains two RfD values: one for drinking water and one for dietary exposure. Because SCDM calculates RfD-based, non-cancer screening concentration benchmarks for both drinking water and dietary exposures, the more conservative value is used; therefore, SCDM uses the drinking water RfD for cadmium.

- Asbestos and Lead – The HRS specifies that a human toxicity factor of 10,000 be assigned to asbestos, lead and lead compounds. Asbestos also receives a Kd value of 1,000, as stated in the HRS.

- Copper – SCDM uses a HEAST water quality standard of 1.3 mg/L to determine an RfD for copper, based on drinking water exposure assumptions of 70 kg body mass, 30 years exposure, and 1L/day ingestion.

- Vanadium – SCDM assigns an RfD that has been identified for vanadium pentoxide as the RfD for vanadium.

2.2 Data Used to Determine Human Toxicity Factor Values and Screening Concentration Benchmarks

Section 2.2 details how data are obtained for determining human toxicity factor (HTF) values and screening concentration benchmarks. RfD, RfC, SF, IUR, lethal dose with 50% mortality (LD50), lethal concentration with 50% mortality (LC50) and effective dose (ED10) values are identified and used to determine the HTF value for each substance according to HRS Section 2.4.1.1. The RfD, RfC, SF, IUR values are also used to determine screening concentration benchmarks (see Section 4.0 of this document).

Non-carcinogenic data (RfD, RfC, LD50 and LC50) and carcinogenic data (IUR, SF and ED10) are selected for each substance according to a hierarchy of references. Of the values selected, the most conservative (i.e., most protective of human health) is used to determine the HTF, regardless of exposure route or whether the value represents a non-cancer or cancer effect.
2.2.1 SF, IUR, RfD and RfC Data Collection

SCDM does not assign RfD or RfC data to radionuclides. SF values (inhalation, oral and external exposure) are obtained for radionuclides from the following references, listed in order of preference:


For all other substances, RfD and RfC values are obtained from the following references, listed in order of preference:


ATSDR provides MRLs for acute (1 – 14 days), intermediate (>14 – 364 days), and chronic (365 days and longer) exposure durations. During SCDM data collection, preference is given to ATSDR values that are based on chronic exposure. Where chronic exposure values are not available, SCDM uses values based on intermediate exposure. Where intermediate MRLs are used in SCDM, the reference provided in the SCDM Appendices is “ATSDR-Int.” SCDM does not use MRLs that are based on acute exposure.

For non-radionuclide substances, SF and IUR values are obtained from the following references, listed in order of preference:

**2.2.2 Weight of Evidence (WOE)**

When available, a carcinogenic risk WOE classification is collected from the same reference that provided the corresponding cancer risk value (e.g., IUR or SF). If only an oral WOE classification is provided for a substance that is identified as carcinogenic via inhalation, the oral WOE is recorded for the inhalation cancer risk value. In some instances, two or more WOE assessments are provided in a single reference. In these cases, the WOE assessment associated with the selected risk value is used; typically, this is the most recent WOE assessment.

**2.2.3 LD₅₀ – Oral, Dermal; LC₅₀ – Inhalation**

When no RfD, RfC, cancer SF with WOE or IUR with WOE are available, SCDM uses an LD₅₀ (oral, dermal) or LC₅₀ (dust and gas inhalation) to assign HTF values. The lowest value is used to determine the HTF. LD₅₀ and LC₅₀ values are not used to calculate screening concentration benchmarks.

SCDM does not assign LD₅₀ and LC₅₀ values to radionuclides. The references used to collect these data for other substances are listed below, in order of preference:


SCDM contains the lowest LD₅₀ or LC₅₀ value for any mammalian species by the oral and dermal exposures, in controlled dose studies, with durations of less than 24 hours. LD₅₀ and LC₅₀ data that are reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM.
2.2.4  \textit{ED}_{10} and Weight-of-Evidence – Oral, Inhalation

When a cancer SF with WOE is not available, SCDM uses \textit{ED}_{10} oral and inhalation values to calculate cancer SF (see Section 3.3 of this methodology document). SCDM does not assign \textit{ED}_{10} values to radionuclides. For all other substances, SCDM uses data from the following references, listed in order of preference for oral and inhalation \textit{ED}_{10} and associated WOEs:


\textit{ED}_{10} data that are reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM.

2.3  Mobility Information

Vapor pressures and Henry’s Law Constants are used to determine the gas migration potential and gas mobility potential for each substance. Water solubility and soil/water distribution coefficients are used to determine ground water mobility factor values. Henry’s Law Constants are also used to determine volatilization half life.

2.3.1  Vapor Pressure

SCDM uses data from the following references to obtain vapor pressures for organic compounds, listed in order of preference:


SCDM uses data from the following references to obtain vapor pressures for non-organic compounds, listed in order of preference:


If a recommended vapor pressure is not provided in the references, SCDM uses a value measured at 25°C. If more than one vapor pressure measured at 25°C is available, SCDM uses the highest value. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If no temperature is specified for all vapor pressure measurements for a substance, SCDM uses the highest value.

If no vapor pressure values are available in any of the references listed or if the referenced value is suspect, a value may be either selected from a data source outside the hierarchy or estimated. For any given substance, suspect values are identified by comparison with other vapor pressure values in SCDM data sources or other sources of chemical property data. The procedures described in Lyman et al. (1990) are used to estimate vapor pressure. RTI (1996) describes the use of these procedures for specific hazardous substances.


For organic substances, if a vapor pressure is not available, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atmosphere (atm) is <25°C, a default vapor pressure of 760 Torr is used with the assumption that the substance is a gas at 25°C.

If no vapor pressure is available for a substance and the normal boiling point is ≥25°C, SCDM assumes that the substance is in a particulate form, rather than a gaseous form, and no vapor pressure is assigned. This assumption is made because the absence of a vapor pressure value often reflects an extremely low and difficult to measure (under standard conditions) value for nongaseous substances.

### 2.3.2 Henry’s Law Constant

SCDM uses data from the following references to obtain Henry’s Law Constants (HLC) for organic compounds, listed in order of preference:


SCDM uses data from the following references to obtain HLC’s for inorganic compounds, listed in order of preference:


If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all Henry’s Law Constants for a substance, SCDM uses the highest value.

### 2.3.3 Water Solubility

Water solubility is used, along with Kd values, to calculate the ground water mobility of hazardous substances that do not meet observed release criteria. All hazardous substances that are available to migrate from sources at a site to the ground water are evaluated for ground water mobility. Water solubility values are also used to assign BCF values for hazardous substances when BCF or Log Kow data are not available.

#### 2.3.3.1 Water Solubility - Organic Substances

SCDM obtains water solubility values for organic substances from the following references, listed in order of preference:


If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all water solubility measurements for a substance, SCDM uses the highest value.

2.3.3.2 Water Solubility – Metals, Metalloids and Radionuclides

SCDM obtains water solubility values for metals and metalloid compounds from the following references, listed in order of preference:


For a metal or metalloid substance, SCDM determines and assigns water solubility as the geometric mean of the highest and lowest water solubility values available for compounds containing the metal or metalloid, as defined in the HRS (see HRS Section 3.2.1.2, Mobility) and described in Section 3.7 of this document.

2.3.4 Soil/Water Distribution Coefficient (Kd); Soil Organic/Carbon Partition Coefficients (Koc and Log Kow)

Kd values are used to calculate ground water mobility for hazardous substances that do not meet observed release criteria. If Kd values are not available, associated Koc and Log Kow values are used to calculate Kd. All
hazardous substances that are available to migrate from sources at the site to ground water are evaluated for ground water mobility.

For organic substances, SCDM calculates the $K_d$ according to HRS Section 3.2.1.2 (Mobility) and the relationship of $K_d = K_{OC} \times f_s$ (see Section 3.6 of this methodology document), where $f_s$ is the sorbent content (fraction of clays plus organic carbon) and $K_{OC}$ is obtained from the following references, listed in order of preference:

- **EPI Suite™ (estimated values)** developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC).
  


- **EPI Suite™ (experimental values)** developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC).
  

- **Estimated as described in Section 3.6 of this methodology document**

When using values from EPI Suite™, SCDM prefers $K_{OC}$ values that are estimated using the Molecular Connectivity Index (MCI) method over $K_{OC}$ values that are estimated by the Log $K_{OW}$ method. When a $K_{OC}$ is not available using the MCI method, SCDM uses the EPI Suite™ $K_{OC}$ values estimated using the Log $K_{OW}$ method. Information regarding collection of Log $K_{OW}$ values is provided in Section 2.5.2 of this methodology document. Section 3.6 (Soil Water Distribution Coefficient [$K_d$]; Soil Organic/Carbon Partition Coefficients [$K_{OC}$]) of this document provides additional information regarding SCDM calculations of $K_d$ and $K_{OC}$ values.

SCDM obtains $K_d$ values for inorganic substances from the following references, listed in order of preference:


- **HRS Section 3.2.1.2 (See Section 3.6 of this methodology document).**

SCDM contains values corresponding to typical subsurface pH (e.g., 6.8).
2.4 Persistence Information

The evaluation of persistence is based primarily on the half-life of hazardous substances in surface water and (for non-radiionuclides) secondarily on the sorption of the hazardous substances to sediments. Persistence information is used to determine the surface water persistence factor value.

2.4.1 Hydrolysis, Biodegradation and Photolysis Half-Lives

SCDM does not assign hydrolysis, biodegradation or photolysis half lives to radionuclides. SCDM obtains hydrolysis, biodegradation and photolysis half-lives for all other substances from the following references, listed in order of preference:


SCDM only uses values that have been measured in water from the CHEMFATE database. SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest value. If no value is available at 25°C, a value determined at a temperature closest to 25°C is selected. If no temperature is specified for all half-life values for a substance, SCDM uses the highest value. If values are obtained from HEDR, SCDM uses only values listed as “first-order.” If multiple values are provided, the highest value is used.

2.4.2 Volatilization Half-Lives

SCDM estimates volatilization half-lives for organic substances in both rivers and lakes, using the equations and procedures described in Section 3.4 of this methodology document. Volatilization half-lives are not collected or estimated for inorganic substances.

2.4.3 Radioactive Half-Lives

SCDM obtains radioactive half-lives for radioactive substances from the following references, listed in order of preference:


2.5 Bioaccumulation Potential Information

BCF values for freshwater and saltwater (one set each for the human food chain and environmental threats) are used to determine bioaccumulation potential factor values (40 CFR Part 300, Appendix A, Section 4.1.3.2.1.3). BCF values are selected based on edible species to determine bioaccumulation potential factor values for the human food chain threat. If BCF data are not available for organic substances, the Log K<sub>OW</sub> is used to determine
bioaccumulation potential factor values. Water solubility data are used if the Log K_{ow} exceeds 6.0, the
substance is inorganic or there is no Log K_{ow}.

2.5.1 Bioconcentration

Bioaccumulation factor values in SCDM are preferentially based on actual measurements of bioconcentration in
aquatic organisms. SCDM used BCF values from the following sources, listed in order of preference:

- U.S. EPA. ECOTOX Database. Environmental Research Laboratory, Duluth, MN.  

  Washington, DC. Contract No. 68-W8-0098.

SCDM uses the highest measured value from ECOTOX. Measured values are preferred over calculated or
estimated values. The Versar reference is a report of literature survey BCF values developed to obtain
preliminary values for use when the initial HRS was being developed. When using data from this reference,
SCDM also prefers the highest measured value to an estimated value. BCF data reported in the references as less
than or greater than a particular value are considered non definitive and are not used in SCDM.

Environmental Threat: For the environmental threat, the highest value from any aquatic organism, regardless of
whether it is consumed by humans, in each reference is used to establish environmental threat BCF values.

Human Food Chain Threat: The highest measured BCF for aquatic organisms typically known to be consumed
by humans is used to obtain the human food chain threat BCF values. Table 1 includes a list of some of the
organisms for which these BCF values may be taken. This list is intended to serve only as a guide to the SCDM
data collector and hence, not all human food chain aquatic organisms are listed. Values from organisms not in
this list may be used provided they are known to be consumed by humans.

Table 1. Examples of Human Food Chain Aquatic Organisms

<table>
<thead>
<tr>
<th>American or Virginia oyster</th>
<th>Carp</th>
<th>Kiyi</th>
<th>Red abalone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asiatic clam</td>
<td>Chinook salmon</td>
<td>Lake trout (siscowet)</td>
<td>Red swamp crayfish</td>
</tr>
<tr>
<td>Atlantic dogwinkle</td>
<td>Channel catfish</td>
<td>Lake whitefish</td>
<td>River salmon</td>
</tr>
<tr>
<td>Atlantic salmon</td>
<td>Clam</td>
<td>Largemouth bass</td>
<td>Rock bass</td>
</tr>
<tr>
<td>Atlantic silverside</td>
<td>Cockle</td>
<td>Limpet</td>
<td>Rough periwinkle</td>
</tr>
<tr>
<td>Bay scallop</td>
<td>Cocho salmon</td>
<td>Lobster</td>
<td>Sauger</td>
</tr>
<tr>
<td>Bent-nosed clam</td>
<td>Common bay mussel</td>
<td>Mangrove snapper</td>
<td>Scallopc</td>
</tr>
<tr>
<td>Bivalve/clam/mussel</td>
<td>Common mirror colored</td>
<td>Marsh snail</td>
<td>Shrimp</td>
</tr>
<tr>
<td>Black abalone</td>
<td>Carp</td>
<td>Mussel</td>
<td>Sole</td>
</tr>
<tr>
<td>Black bullhead</td>
<td>Common shrimp</td>
<td>Netted dogwhelk</td>
<td>Spot</td>
</tr>
<tr>
<td>Black crappie</td>
<td>Crab</td>
<td>Northern anchovy</td>
<td>Striped bass</td>
</tr>
<tr>
<td>Black mussel</td>
<td>Crayfish</td>
<td>Northern krill</td>
<td>Striped mullet</td>
</tr>
<tr>
<td>Blue crab</td>
<td>Dungeness or edible crab</td>
<td>Northern pike</td>
<td>Swan mussel</td>
</tr>
<tr>
<td>Bluegill</td>
<td>Eel</td>
<td>Oyster</td>
<td>Taiwan abalone</td>
</tr>
<tr>
<td>Bony fishes</td>
<td>Filefish</td>
<td>Pilchard sardine</td>
<td>Tong sole</td>
</tr>
<tr>
<td>Brook silverside</td>
<td>Flounder</td>
<td>Pinfish</td>
<td>Topmouth gudgeon (golden shiner)</td>
</tr>
<tr>
<td>Brook trout</td>
<td>Giant gourami</td>
<td>Pink salmon</td>
<td>White mullet</td>
</tr>
<tr>
<td></td>
<td>Green sunfish</td>
<td>Porgy</td>
<td>White sand mussel</td>
</tr>
</tbody>
</table>
2.5.2 **Octanol/Water Partition Coefficient (Log $K_{OW}$)**

Log $K_{OW}$ values are used to determine the bioaccumulation potential factor value for a hazardous substance for which BCF data are not available. SCDM may also use the log $K_{OW}$ to estimate a log $K_{OC}$ when a $K_{OC}$ is not available (see Sections 2.3.4 and 3.2 of this methodology document). SCDM obtains n-octanol/water (log $K_{OW}$, also referred to as Log P) values from the following sources, listed in order of preference:


SCDM uses experimental values; estimated or calculated values are not used. If values are obtained from CHEMFATE, the recommended values are used.

2.5.3 **Water Solubility**

Water solubility values are used to assign a bioaccumulation potential factor value for hazardous substances when BCF or log $K_{OW}$ data are not available. See Sections 2.3.3.1 (Water Solubility – Organic Substances) and 2.3.3.2 (Water Solubility – Metals, Metalloids and Radionuclides) of this methodology document for the data collection protocol and guidance on water solubility values.

2.6 **Ecotoxicity Parameters**

Ecotoxicity data are used in the HRS scoring system to determine the Ecotoxicity Factor values (HRS; 40 CFR Part 300, Appendix A, Section 4.1.4.2.1.1). SCDM uses acute and chronic freshwater and saltwater criteria, and only uses those values specifically stated as criteria. If criteria are not available, then LC$_{50}$ data are used.

2.6.1 **Acute and Chronic Freshwater and Saltwater Criteria - CCC, CMC**

The HRS (Section 4.1.4.2.1.1, Ecosystem Toxicity) uses the EPA Ambient Water Quality Criteria (AWQC) and Ambient Aquatic Life Advisory Concentrations (AALAC) for assigning ecosystem toxicity factor values. The
acute and chronic AWQC have been replaced by a new set of criteria, and the AALAC values no longer exist. The new criteria replacing the AWQC for both freshwater and saltwater are labeled as (1) Criteria Maximum Concentration (CMC), to be used in place of what was previously acute AWQC, and (2) Criteria Continuous Concentration (CCC), to be used in place of what was previously chronic AWQC. These new values closely correspond to the old acute and chronic AWQC values, respectively; however, some values have been re-derived using different methodology. Therefore, the resulting values must be used as directed by the EPA. Many of the CMC and CCC values have associated endnotes regarding how the value was derived and how it should be used. Some CMC and CCC values are baseline values that must be adjusted using the information specified in the endnotes. The CMC and CCC values are taken from:


2.6.2 **LC50 - Freshwater, Saltwater**

SCDM obtains LC50 data from the ECOTOX database for both freshwater and saltwater.


SCDM uses the lowest acute LC50 value found for any aquatic organism in the specified environment with an acute exposure duration of \( \geq 1 \) day and \( \leq 4 \) days. When no duration or environment is given, LC50 values are not entered into SCDM.

2.7 **Regulatory Benchmarks**

The HRS assigns extra weight to targets with exposure to hazardous substances at levels that are at or above regulatory benchmark values. This section describes the sources for regulatory limits that the HRS uses as health-based or ecological-based benchmarks.

2.7.1 **National Ambient Air Quality Standards (NAAQS)**

National Ambient Air Quality Standards (NAAQS) are used to establish Level I concentrations. Targets exposed to concentrations at or above the NAAQS are scored as Level I targets. SCDM uses data from the following source to obtain NAAQS:


2.7.2 **National Emissions Standards for Hazardous Air Pollutants (NESHAPs)**

National Emission Standards for Hazardous Air Pollutants (NESHAPs) are used to establish Level I concentrations. Targets exposed to concentrations at or above NESHAPs are scored as Level I targets. SCDM uses data from the following source to obtain NESHAPs and uses only those values that are reported in ambient concentration units (µg/m³):

2.7.3 Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs)

Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs) are used to establish Level I concentrations. Targets exposed to concentrations at or above MCLs and MCLGs are scored as Level I targets. SCDM uses data from the following sources for MCLs and MCLGs:


SCDM uses only MCLs that are reported in units of concentration (mg/L, μg/L or pCi/L) and only non-zero MCLGs that are reported in units of concentration (mg/L or μ/L). For substances where multiple values are listed, SCDM uses the lowest value. For substances where both MCLs and MCLGs are provided but are different, SCDM selects the lower of the two values.

2.7.4 FDA Action Levels (FDAALs)

Food and Drug Administration Action Levels (FDAAL) are used to establish Level I concentrations. Targets exposed to concentrations at or above FDAALs are scored as Level I targets. SCDM contains FDAALs for fish and shellfish only, and obtains the FDAAL values from the following reference:


2.7.5 Ecological Based Benchmarks

See Section 2.6.1 of this document for information regarding acute CMC and chronic CCC for freshwater and saltwater.

2.7.6 Uranium Mill Tailings Radiation Control Act Standards (UMTRCA)


2.8 Physical Properties

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point and melting point. SCDM applies yes/no flags to classify physical property data into the four substance categories defined below.
**Organic Substances (“Organic”):** “Y” indicates that the substance is organic, and “N” indicates an inorganic substance. This flag is used to determine factor values for ground water mobility and bioaccumulation potential. Volatile and semivolatile organics are indicated. These flags influence the SCDM calculation of $K_d$ values.

**Metal-Containing Substances (“Metal Contain”):** “Y” indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. “N” indicates that the substance is not, or does not contain, a metal or metalloid. This flag is used to determine factor values for ground water mobility and surface water persistence.

**Radioactive Isotope (“Radionuclide”):** “Y” indicates that the substance is a specific radioactive isotope, and “N” indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag is used to determine factor values for human toxicity, ecosystem toxicity and surface water persistence.

**Radioactive Element (“Rad. Element”):** “Y” indicates that the substance is a radioactive element, and “N” indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag determines whether or not the HRS factors and benchmarks are printed in Appendix A.

### 2.8.1 Chemical Formula, Boiling Point and Melting Point

Chemical formula, boiling point and melting point data are extracted for inorganic substances, from the following sources in order of preference:


Chemical formula, boiling point and melting point data are extracted for all other substances, from the following sources in order of preference:


2.8.2 Molecular Weight

Molecular weight data are collected for inorganic substances, from the following sources in order of preference:


Molecular weight data are collected for all other substances, from the following sources in order of preference:


2.8.3 Density

Density data are collected for inorganic substances, from the following sources in order of preference:

Density data are collected for all other substances, from the following sources in order of preference:


3.0 CALCULATION OF INTERIM VALUES

SCDM calculates specific chemical properties for some of the following cases:
- when all preferred references do not contain a property value for a given chemical
- the property value or values from a given reference cannot be used because they are suspect or
- the EPA specifies that a value be calculated

3.1 RfC to RfD_{inhal}

SCDM contains RfD values for oral toxicity and RfC values for inhalation toxicity that are used to determine HTF values and screening concentration benchmarks. SCDM must convert RfC to RfD_{inhal}, for use in these determinations. RfC values are converted from concentrations into inhalation dosages (RfD_{inhal}) values for determining HTF values using the following equation:

\[
RFD_{inhal} = \frac{RFC \times IR \times AR}{BM}
\]

Where:
- \(RFD_{inhal}\) = Calculated Reference Dose in Air (mg/kg-day)
- \(RFC\) = Reference Concentration in Air (mg/m^3)
- \(IR\) = Inhalation Rate (20 m^3/day)
- \(AR\) = Absorption (100% assumed unless otherwise specified)
- \(BM\) = Adult Body Mass (70 kg)

Equation (1) is used to convert RfCs to inhalation RfDs. The resulting RfD_{inhal} values are used to determine HTF values (see HRS Section 2.4.1.1, Table 2-4 [40 CFR Part 300]). If the reference source used to provide the RfD or RfC does not provide a corresponding absorption, it is assumed to be 100.

3.2 IUR to Inhalation Slope Factor

SCDM contains slope factors for oral toxicity and IUR values for inhalation toxicity. IUR values are converted into inhalation slope factors (SF_{inhal}) for use in determining HTF values. SCDM converts IUR values to calculated SF_{inhal} before assigning HTF values, using the following equation:

\[
SF_{inhal} = \frac{IUR \times BM \times CF}{IR \times AR}
\]

Where:
- \(SF_{inhal}\) = Cancer Slope Factor (mg/kg-day)^{-1}
- \(IUR\) = Inhalation Unit Risk (µg/m^3)^{-1}
- \(BM\) = Adult Body Mass (70 kg)
- \(CF\) = Conversion Factor (1,000 µg/mg)
- \(IR\) = Inhalation Rate (20 m^3/day)
- \(AR\) = Absorption (100% assumed unless otherwise specified)

Equation (2) is used to convert the IUR value to an inhalation cancer SF, and the resulting inhalation cancer SF is evaluated with a corresponding WOE (see Section 2.2.2.1 above) to assign an HTF value based on HRS Table 2-4 (40 CFR Part 300).
3.3 Using ED10 to estimate a Slope Factor for either oral or inhalation pathways

SCDM uses slope factors and IUR values to determine human toxicity factor values and screening concentration benchmarks. In cases where a slope factor and/or IUR is not available for a substance, SCDM uses ED10 values, when available, to calculate oral and inhalation slope factors ($S_{\text{oral}}$ and $S_{\text{inhal}}$), as follows:

$$S_{\text{oral}} = \frac{1}{(6 \times \text{ED10}_{\text{oral}})} \quad (3)$$

$$S_{\text{inhal}} = \frac{1}{(6 \times \text{ED10}_{\text{inhal}})} \quad (4)$$

3.4 Volatilization Half-Life

SCDM estimates the volatilization half-life in surface water for organic substances using Equation 5 (presented as Equation 15-12 in the “Handbook of Chemical Property and Estimation Methods,” Lyman, et al.\(^1\)) In this method, the volatilization half-life ($T_{1/2}$) can be expressed as follows:

$$T_{1/2} = \left[ \frac{Z \times \ln 2}{K_L \times \text{hr}} \right]$$

*Where:*

- $Z =$ Mean water body depth (cm)
- $K_L =$ Overall liquid-phase mass transfer coefficient
- $\ln 2 =$ Natural logarithm of 2 (~0.693147)

The following expression gives the overall liquid-phase mass transfer coefficient:

$$K_L = \frac{(H/RT)k_g \times k_l}{(H/RT)k_g + k_l} \text{ cm/hr} \quad (6)$$

*Where:*

- $H =$ Henry’s Law constant (atm·m³/mol)
- $R =$ Universal gas constant (8.2 × 10⁻⁵ atm·m³/mol·K)
- $T =$ Temperature (K; °C + 273)
- $k_g =$ Gas-phase exchange coefficient
- $k_l =$ Liquid-phase exchange coefficient

The gas-phase exchange coefficient expression depends on the molecular weight (MW) of the compound.

- If MW is <65 g/mol, the following equation is used:

  $$k_g = 3,000 \times (18 / \text{MW})^{1/2} \text{ cm/hr} \quad (7)$$

- If MW is ≥65 g/mol, the following equation is used:

\[ k = 1,137.5 \times (V_{wind} + V_{curr})(18 / MW)^{1/2} \text{ cm/hr} \] (8)

Where:

\[ \begin{align*}
V_{wind} &= \text{Wind velocity (m/sec)} \\
V_{curr} &= \text{Current velocity (m/sec)}
\end{align*} \]

The liquid-phase exchange coefficient also depends on the molecular weight of the compound.

- If MW is $< 65$ g/mol, the following equation is used:

\[ k_1 = 20 \times (44 / MW)^{1/2} \text{ cm/hr} \] (9)

- If MW is $\geq 65$ g/mol, the expression also depends on the wind and current velocities; the following equation is used when $V_{wind} \leq 1.9$ m/sec and MW is $\geq 65$ g/mol:

\[ k_1 = 23.51 \times (V_{curr}^{0.969} / Z^{0.673}) \times (32 / MW)^{1/2} \text{ cm/hr} \] (10)

The following equation is used when $V_{wind} > 1.9$ m/sec and $\leq 5$ m/sec, and MW is $\geq 65$ g/mol:

\[ k_1 = 23.51 \times (V_{curr}^{0.969} / Z^{0.673}) \times (32 / MW)^{1/2} \times e^{0.526(V_{wind} - 1.9)} \text{ cm/hr} \] (11)

No liquid-phase exchange coefficient equation is provided in Thomas (1990) for wind velocities $> 5$ m/sec.

Combining Equations (5), (6), (7), and (9) into a single equation for estimating volatilization half-life ($T_{1/2}$) for compounds with MW $< 65$ g/mol gives the following equation:

\[ T_{1/2} = Z \times \ln 2 \times \left\{ [1 / 20] \times (MW / 44)^{1/2} \right\} + [(RT / H \times 3000) \times (MW / 18)^{1/2}] \text{ hr} \] (12)

The following equation, combining Equations (5), (6), (8), and (10), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW $\geq 65$ g/mol if the wind velocity is $\leq 1.9$ m/sec:

\[ T_{1/2} = Z \times \ln 2 \times \left\{ [(Z^{0.673} / 23.51 \times V_{curr}^{0.969}) \times (MW / 32)^{1/2}] + [(RT / H \times 1,137.5) \times (V_{wind} + V_{curr}) \times (MW / 18)^{1/2}] \right\} \text{ hr} \] (13)

The following equation, combining Equations (5), (6), (8), and (11), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW $\geq 65$ g/mol if the wind velocity is $> 1.9$ m/sec and $\leq 5$ m/sec:

\[ T_{1/2} = Z \times \ln 2 \times \left\{ [(Z^{0.673} / 23.51 \times V_{curr}^{0.969}) \times (MW / 32)^{1/2}] e^{0.526(1.9 - V_{wind})} + [(RT / H \times 1,137.5) \times (V_{wind} + V_{curr}) \times (MW / 18)^{1/2}] \right\} \text{ hr} \] (14)
If $H < 10^{-7}$ atm·m$^3$/mol, the substance is less volatile than water, and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, p. 15-15), and no volatilization half-life is estimated for rivers or lakes.

### 3.4.1 Volatilization Half-Life for Rivers, Oceans, Coastal Tidal Waters and the Great Lakes

To calculate the volatilization half-life for rivers, oceans, coastal tidal waters and the Great Lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 1 m/sec. Using these values, Equations (12) and (14) reduce to the following:

- If $MW < 65$ g/mol:
  \[
  T_{1/2} = 2.89 \times [(0.05 \times (MW/44)^{1/2}) + (8.1 \times 10^{-6} / H) \times (MW/18)^{1/2}] \text{ days} \tag{15}
  \]

- If $MW \geq 65$ g/mol:
  \[
  T_{1/2} = 2.89 \times [(0.185 \times (MW/32)^{1/2}) + (3.6 \times 10^{-6} / H) \times (MW/18)^{1/2}] \text{ days} \tag{16}
  \]

Where:
- $H = \text{Henry’s Law Constant (atm·m}^3$/mol$)$
- $MW = \text{Molecular Weight (g/mol)}$

### 3.4.2 Volatilization Half-Life for Lakes

To calculate the volatilization half-life for lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 0.05 m/sec. Using these values, Equations (12) and (13) reduce to the following:

- If $MW < 65$ g/mol:
  \[
  T_{1/2} = 2.89 \times [(0.05 \times (MW/44)^{1/2}) + (8.1 \times 10^{-6} / H) \times (MW/18)^{1/2}] \text{ days} \tag{17}
  \]

- If $MW \geq 65$ g/mol:
  \[
  T_{1/2} = 2.89 \times [(0.185 \times (MW/32)^{1/2}) + (3.9 \times 10^{-6} / H) \times (MW/18)^{1/2}] \text{ days} \tag{18}
  \]

Where:
- $H = \text{Henry’s Law Constant (atm·m}^3$/mol$)$
- $MW = \text{Molecular Weight (g/mol)}$

### 3.5 Overall Half-Lives

#### 3.5.1 Overall Half-Lives for Non-radionuclides

Overall half-lives are estimated for non-radioactive substances, in rivers and lakes, as follows:

\[
\text{HALF\_LAK} = \frac{1}{\text{HALF}_{\text{FL}} + \text{HALF}_{\text{FL}} + \text{HALF}_{\text{FL}} + \text{HALF}_{\text{FL}}} \tag{19}
\]
Where:
HHHALFL = Hydrolysis half-life in lakes
BHHALFL = Biodegradation half-life in lakes
PHHALFL = Photolysis half-life in lakes
VHALFL = Volatilization half-life in lakes

\[
HALF_{RIV} = \frac{1}{HHHALFR + 1/BHALFR + 1/PHHALFR + 1/VHALFL}
\]

Where:
HHHALFR = Hydrolysis half-life in rivers
BHHALFR = Biodegradation half-life in rivers
PHHALFR = Photolysis half-life in rivers
VHALFR = Volatilization half-life in rivers

3.5.2 Overall Half-Lives for Radionuclides

SCDM estimates overall half-lives of radionuclides in rivers and lakes as follows (this calculation is similar to the equation used for non radioactive substances, but considers only radioactive half life and volatilization half life):

\[
HALF_{R,LAK} = \frac{1}{1/RHALFL + 1/VHALFL}
\]

Where:
RHALFL = Radioactive half-life in lakes
VHALFL = Volatilization half-life in lakes

\[
HALF_{R,RIV} = \frac{1}{1/RHALFR + 1/VHALFR}
\]

Where:
RHALFR = Radioactive half-life in rivers
VHALFR = Volatilization half-life in rivers

3.6 Soil Water Distribution Coefficient (K_d); Soil Organic/Carbon Partition Coefficients (K_{oc})

In the evaluation of the ground water migration pathway, a hazardous substance that does not meet the criteria for an observed release is assigned a mobility factor value from HRS Table 3-8 (Ground Water Mobility Factor Values) based on its K_d value and its water solubility value. K_d values that are not available in the references listed in Section 2.3.4 of this methodology document are calculated as detailed below:

HRS Section 3.2.1.2 (Mobility) states:
For any hazardous substance that does not meet the criteria for an observed release by chemical analysis to at least one of the aquifers, assign that hazardous substance a mobility factor value from Table 3-8 for the aquifer being evaluated, based on its water solubility and distribution coefficient (K_d).... For any hazardous substance that is organic and that does not meet the criteria for an observed release by chemical analysis, establish a distribution coefficient for that hazardous substance as follows:

Estimate K_d range for the hazardous substance using the following equation:

\[ K_d = (K_{OC})(f_S) \]  

Where:
- \( K_{OC} \) = Soil-water partition coefficient for organic carbon for the hazardous substance
- \( f_S \) = Sorbent content (fraction of clays plus organic carbon) in the subsurface

* Use \( f_S \) values of 0.03 and 0.77 in the above equation to establish the upper and lower values of the K_d range for the hazardous substance.
* Calculate the geometric mean of the upper and lower K_d range values. Use this geometric mean as the distribution coefficient in assigning the hazardous substance a mobility factor value from [HRS] Table 3-8.

When a \( K_{OC} \) is not available to calculate K_d values, SCDM uses the Log P or Log K_{ow} to estimate \( K_{OC} \) values. To perform this calculation, SCDM uses the relationship determined by Di’Toro (1985) for semi-volatile organic compounds:

\[ \log K_{OC} = 0.00028 + (0.983 \log K_{ow}) \]  

For volatile organic compounds, chlorinated benzenes, and certain chlorinated pesticides, SCDM uses the relationship derived in the Soil Screening Guidance Technical Background Document (EPA, 1996):

\[ \log K_{OC} = 0.0784 + (0.7919 \log K_{ow}) \]  

### 3.7 Water solubility for metals

If a water solubility value is not available for metal substances, it is calculated as the geometric mean of the highest water solubility and lowest water solubility of substances containing the metal, using the following equation:

\[ \text{Geometric Mean Solubility} = \sqrt{\text{low water solubility} \times \text{high water solubility}} \]
4.0 SCREENING CONCENTRATION BENCHMARKS

Section 4 details the equations and exposure assumptions that are used to determine screening concentration benchmarks for the substances contained in SCDM. The sources of data and determination of the substance-specific values used in these equations are detailed in Sections 2.0 and 3.0 of this methodology document.

4.1 Screening Concentration Benchmarks for the Air Migration Pathway

The following equations are used to determine air inhalation screening concentration benchmarks for the air migration pathway. The benchmarks use exposure parameters and factors that represent Reasonable Maximum Exposure (RME) conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA’s Risk Assessment Guidance for Superfund, Part B (1991) and Risk Assessment Guidance for Superfund, Part F (2009). General equations are provided in Section 4.1.1 (non-carcinogenic benchmarks) and Section 4.1.2 (carcinogenic benchmarks). An equation specific for asbestos is provided in Section 4.1.3. Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and trichloroethylene (TCE), are provided in Section 4.1.4; these equations are taken from EPA’s Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites. Equations used for radionuclides are provided in Section 4.1.5.

4.1.1 Non-carcinogenic – Air, Inhalation

\[
SC_{nc-air} = \frac{THQ \times (AT \times ED) \times \left(\frac{1000 \ \mu g}{mg}\right)}{EF \times ED \times ET \times \left(\frac{1 \ \text{day}}{24 \ \text{hours}}\right) \times \frac{1}{RfC}}
\]

(27)

Where:
- \(SC_{nc-air}\) = Air Inhalation Screening Concentration, Non-Carcinogenic (µg/m³)
- \(THQ\) = Target hazard quotient (=1), unitless
- \(AT\) = Averaging time (365 days/year)
- \(ED\) = Exposure duration (30 years)
- \(EF\) = Exposure frequency (350 days/year)
- \(ET\) = Exposure time (24 hours/day)
- \(RfC\) = Inhalation reference concentration (mg/m³)

Using the exposure assumptions listed above, Equation (27) can be simplified as:

\[
SC_{nc-air} = 1042.857 \times RfC
\]

(28)

4.1.2 Carcinogenic – Air, Inhalation

\[
SC_{c-air} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times \left(\frac{1 \ \text{day}}{24 \ \text{hours}}\right) \times IUR}
\]

(29)

Where:
- \(SC_{c-air}\) = Air Inhalation Screening Concentration, Carcinogenic (µg/m³)
TR = Target risk (1 x 10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
ED = Exposure duration (30 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk (µg/m^3)^{-1}

Using the exposure assumptions listed above, Equation (29) can be simplified as:

\[ SC_{c-air} = \frac{2.433 \times 10^{-6}}{IUR} \]  

(30)

### 4.1.3 Carcinogenic – Air, Inhalation – Asbestos

\[ SC_{c-air-asbestos} (fibers/mL) = \frac{TR}{IUR \times TWF} \]  

(31)

Where:

- \( SC_{c-air-asbestos} \) = Air Inhalation Screening Concentration, Carcinogenic, Asbestos (fibers/mL)
- \( TR \) = Target risk (1 x 10^{-6}) (unitless)
- \( IUR \) = Inhalation Unit Risk (fibers/mL)^{-1}
- \( TWF \) = Time Weighting Factor = 350/365 = 0.96

### 4.1.4 Carcinogenic through a Mutagenic Mode of Action – Air, Inhalation

\[ SC_{mu-air} = \frac{TR \times (AT \times LT)}{EF \times ET \times \left( \frac{1 \text{ day}}{24 \text{ hours}} \right) \times \left[ (ED_{0-2} \times IUR \times 10) + (ED_{2-6} \times IUR \times 3) \right.} \]
\[ + (ED_{6-16} \times IUR \times 3) + (ED_{16-30} \times IUR \times 1) \]  

(32)

Where:

- \( SC_{mu-air} \) = Air Inhalation Screening Concentration, Carcinogenic – Mutagenic Mode of Action (µg/m^3)
- \( TR \) = Target risk (1 x 10^{-6}) (unitless)
- \( AT \) = Averaging time (365 days/year)
- \( LT \) = Lifetime (70 years)
- \( ED_{0-2} \) = Exposure duration (2 years)
- \( ED_{2-6} \) = Exposure duration (4 years)
- \( ED_{6-16} \) = Exposure duration (10 years)
- \( ED_{16-30} \) = Exposure duration (14 years)
- \( EF \) = Exposure frequency (350 days/year)
- \( ET \) = Exposure time (24 hours/day)
- \( IUR \) = Inhalation unit risk (µg/m^3)^{-1}

Using the exposure assumptions listed above, Equation (32) can be simplified as:
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\[ SC_{mu-air} = \frac{9.605 \times 10^{-7}}{IUR} \]  

(33)

4.1.4.1 Vinyl Chloride – Air, Inhalation

\[ SC_{mu-vc} = \frac{TR}{IUR + \left[ \frac{IUR \times EF \times ED \times ET \times (1 \text{ day} / 24 \text{ hours})}{(AT \times LT)} \right]} \]  

(34)

Where:

- \( SC_{mu-vc} \) = Air Inhalation Screening Concentration, Vinyl Chloride (µg/m³)
- \( TR \) = Target risk (1 x 10⁻⁶)
- \( AT \) = Averaging time (365 days/year)
- \( LT \) = Lifetime (70 years)
- \( ED \) = Exposure duration (30 years)
- \( EF \) = Exposure frequency (350 days/year)
- \( ET \) = Exposure time (24 hours/day)
- \( IUR \) = Inhalation unit risk (µg/m³⁻¹)

Using the exposure assumptions listed above, Equation (34) can be simplified as:

\[ SC_{mu-vc} = \frac{7.090 \times 10^{-7}}{IUR} \]  

(35)

4.1.4.2 Trichloroethylene – Air, Inhalation

The following three steps are used to calculate an air inhalation cancer screening concentration benchmark for TCE.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney IUR and the mutagenic equation provided below.

\[ SC_{mu-tce} = \frac{TR \times (AT \times LT)}{EF \times ET \times (1 \text{ day} / 24 \text{ hours}) \times \left[ (ED_{0-2} \times IUR_{kidney} \times 10) + (ED_{2-6} \times IUR_{kidney} \times 3) + (ED_{6-10} \times IUR_{kidney} \times 3) + (ED_{16-30} \times IUR_{kidney} \times 1) \right]} \]  

(36)

Where:

- \( SC_{mu-tce} \) = Air Inhalation Screening Concentration, Carcinogenic–Mutagenic Mode of Action (µg/m³)
- \( TR \) = Target risk (1 x 10⁻⁶) (unitless)
- \( AT \) = Averaging time (365 days/year)
- \( LT \) = Lifetime (70 years)
- \( ED_{0-2} \) = Exposure duration (2 years)
- \( ED_{2-6} \) = Exposure duration (4 years)
- \( ED_{6-10} \) = Exposure duration (10 years)
- \( ED_{16-30} \) = Exposure duration (14 years)
- \( EF \) = Exposure frequency (350 days/year)
- \( ET \) = Exposure time (24 hours/day)
$IUR_{kidney} = \text{Inhalation unit risk, kidney (µg/m}^3\text{)}^{-1}$

Using the exposure assumptions listed above, Equation (36) can be simplified as:

$$SC_{m-air} = 9.61 \times 10^{-7} / IUR_{kidney}$$ (37)

**Step 2.** A cancer SC is calculated using the non-Hodgkin’s lymphoma (NHL) and liver cancer IUR and the cancer equation provided below.

$$SC_{c-tce} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times (1 \text{ day}/24 \text{ hours}) \times IUR_{NHL \text{ and Liver}}}$$ (38)

Where:

- $SC_{c-tce}$ = Air Inhalation Screening Concentration, Carcinogenic (µg/m$^3$)
- $TR$ = Target risk (1 x $10^{-6}$) (unitless)
- $AT$ = Averaging time (365 days/year)
- $LT$ = Lifetime (70 years)
- $ED$ = Exposure duration (30 years)
- $EF$ = Exposure frequency (350 days/year)
- $ET$ = Exposure time (24 hours/day)
- $IUR_{NHL \text{ and liver}}$ = Inhalation unit risk, NHL and liver (µg/m$^3$)$^{-1}$

Using the exposure assumptions listed above, Equation (38) can be simplified as:

$$SC_{c-air} = 2.44 \times 10^{-6} / IUR_{NHL \text{ and liver}}$$ (39)

**Step 3.** A cumulative result of both the mutagenic and cancer screening concentrations calculated in Steps 1 and 2 above is then generated, and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{mu-c-tce} = \frac{1}{\left(\frac{1}{SC_{m-air}} + \frac{1}{SC_{c-air}}\right)}$$ (40)

Substituting the simplified equations provided above, the following is an alternative equation for calculating Step 3 results:

$$SC_{mu-c-tce} = \frac{1}{1.04 \times 10^6 IUR_{kidney} + 4.10 \times 10^5 IUR_{NHL \text{ and Liver}}}$$ (41)
4.1.5 Carcinogenic – Air, Inhalation, Radionuclides

\[
SC_{c-air-rad} = \frac{TR}{ET \times \left( \frac{1 \text{ day}}{24 \text{ hr}} \right) \times EF \times ED \times SF_i \times IFA_{r-ad}}
\]  

Where:

- \( SC_{c-air-rad} \) = Air inhalation screening concentration benchmark – radiochemical (pCi/m³)
- \( SF_i \) = Slope factor – inhalation, radiochemical – substance specific (pCi)^{-1}
- \( TR \) = Target risk (1 x 10^{-6}), unitless
- \( ET \) = Exposure time – resident (24 hours/day)
- \( EF \) = Exposure frequency – resident (350 days/year)
- \( ED \) = Exposure duration – resident (30 years)
- \( IRA_c \) = Inhalation rate – resident child (10 m³/day)
- \( ED_{c} \) = Exposure duration – resident child (6 years)
- \( ED_{r-a} \) = Exposure duration – resident adult (24 years)
- \( IRA_{r-a} \) = Inhalation rate – resident adult (20 m³/day)
- \( IFA_{r-ad} \) = Age-adjusted inhalation factor (18 m³/day)

Using the exposure assumptions listed above, Equation (42) can be simplified as:

\[
SC_{c-air-rad} = 5.29 \times 10^{-12} / SF_i
\]  

4.2 Screening Concentration Benchmarks for the Soil Exposure Pathway

The following equations are used to determine soil ingestion screening concentration benchmarks for the soil exposure pathway. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA’s Risk Assessment Guidance for Superfund, Part B (1991). General equations are provided in Section 4.2.1 (non-carcinogenic benchmarks) and Section 4.2.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 4.2.3; these equations are taken from EPA’s Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites. Equations used for radionuclides are provided in Section 4.2.4. When determining soil ingestion screening concentration benchmarks for arsenic, the SF and RfD are multiplied by a relative bioavailability adjustment (RBA) factor of 0.6 (EPA Guidance for Evaluating the Oral Bioavailability of Metals in Soils for Use in Human Health Risk Assessment).

4.2.1 Non-carcinogenic – Soil, Ingestion

\[
SC_{res-sol-nc-ing} = \frac{THQ \times AT \times ED_C \times BM_C}{EF \times ED_C \times \left( \frac{1}{RfD} \right) \times IRS_C \times 10^{-6} \text{ kg/mg}}
\]  

Where:

- \( SC_{res-sol-nc-ing} \) = Soil Screening Concentration, Non-Carcinogenic (mg/kg)
Using the exposure assumptions listed above, Equation (44) can be simplified as:

\[ SC_{res-sol-ca-ing} = 78214.29 \times RfD \]  

(45)

### 4.2.2 Carcinogenic – Soil, Ingestion

\[
SC_{res-sol-ca-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6} \text{ kg}}{\text{mg}}} 
\]

(46)

Where:

- \( SC_{res-sol-ca-ing} \) = Soil Screening Concentration, Carcinogenic (mg/kg)
- \( IFS \) = Soil ingestion rate – resident, age adjusted \([= (114 \text{ mg-year}) / (\text{kg-day})]\), calculated as:

\[
IFS = \left( \frac{ED_c \times IRS_c}{BM_c} \right) + \left[ \frac{(ED_r - ED_c) \times IRS_a}{BM_a} \right] 
\]

- \( SF \) = Chronic oral cancer slope factor (mg/kg-day)^{-1}
- \( TR \) = Target risk \((= 1 \times 10^{-6})\)
- \( AT \) = Averaging time – resident \((= 365 \text{ days/year})\)
- \( LT \) = Lifetime \((= 70 \text{ years})\)
- \( EF \) = Exposure frequency – resident \((= 350 \text{ days/year})\)
- \( ED_c \) = Exposure duration – resident child \((= 6 \text{ years})\)
- \( ED_r \) = Exposure duration – resident \((= 30 \text{ years})\)
- \( IRS_a \) = Resident soil ingestion rate – adult \((= 100 \text{ mg/day})\)
- \( IRS_c \) = Resident soil ingestion rate – child \((= 200 \text{ mg/day})\)
- \( BM_a \) = Body mass – adult \((= 70 \text{ kg})\)
- \( BM_c \) = Body mass – child \((= 15 \text{ kg})\)

Using the exposure assumptions listed above, Equation (46) can be simplified as:

\[ SC_{res-sol-ca-ing} = \frac{0.64}{SF} \]  

(47)

### 4.2.3 Carcinogenic through a Mutagenic Mode of Action – Soil, Ingestion

\[
SC_{res-sol-mu-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6} \text{ kg}}{\text{mg}}} 
\]

(48)
Where:

\( SC_{\text{res-sol-mu-ing}} \) = Soil Screening Concentration, Carcinogenic – Mutagenic Mode of Action (mg/kg)

\( IFSM \) = Mutagenic soil ingestion rate – resident, age adjusted \([= (489.5 \text{ mg-year}) / (\text{kg-day})]\), calculated as:

\[
\frac{ED_{0-2} \times IRS_c \times 10}{BM_c} + \frac{ED_{2-6} \times IRS_c \times 3}{BM_a} + \frac{ED_{6-16} \times IRS_a \times 3}{BM_a} + \frac{ED_{16-30} \times IRS_a \times 1}{BM_a}
\]

\( SF \) = Chronic oral cancer slope factor (mg/kg-day)\(^1\)

\( TR \) = Target risk \((= 1 \times 10^{-6})\)

\( AT \) = Averaging time – resident \((= 365 \text{ days/year})\)

\( LT \) = Lifetime \((= 70 \text{ years})\)

\( EF \) = Exposure frequency – resident \((= 350 \text{ days/year})\)

\( ED_{0-2} \) = Exposure duration – resident ages 0-2 \((= 2 \text{ years})\)

\( ED_{2-6} \) = Exposure duration – resident ages 2-6 \((= 4 \text{ years})\)

\( ED_{6-16} \) = Exposure duration – resident ages 6-16 \((= 10 \text{ years})\)

\( ED_{16-30} \) = Exposure duration – resident ages 16-30 \((= 14 \text{ years})\)

\( IRS_a \) = Resident soil ingestion rate – adult \((= 100 \text{ mg/day})\)

\( IRS_c \) = Resident soil ingestion rate – child \((= 200 \text{ mg/day})\)

\( BM_a \) = Body mass – adult \((= 70 \text{ kg})\)

\( BM_c \) = Body mass – child \((= 15 \text{ kg})\)

Using the exposure assumptions listed above, Equation (48) can be simplified as:

\[
SC_{\text{res-sol-mu-ing}} = \frac{0.149}{SF}
\]  

\[ (49) \]

4.2.3.1 Vinyl Chloride – Soil, Ingestion

\[
SC_{\text{res-sol-ca-vc-ing}} = \frac{TR}{\left( \frac{SF \times EF \times IFS \times 10^{-6} \text{ kg}}{mg \times AT \times LT} \right) + \left( \frac{SF \times IRS_c \times 10^{-6} \text{ kg}}{mg \times BM_c} \right)}
\]  

\[ (50) \]

Where:

\( SC_{\text{res-sol-ca-vc-ing}} \) = Soil Screening Concentration, Vinyl Chloride (mg/kg)

\( IFS \) = Soil ingestion rate – resident, age adjusted \([= (114 \text{ mg-year}) / (\text{kg-day})]\), calculated as:

\[
\frac{ED_c \times IRS_c}{BM_c} + \frac{(ED_r - ED_c) \times IRS_a}{BM_a}
\]

\( SF \) = Chronic oral cancer slope factor (mg/kg-day)\(^1\)

\( TR \) = Target risk \((= 1 \times 10^{-6})\)

\( AT \) = Averaging time – resident \((= 365 \text{ days/year})\)

\( LT \) = Lifetime \((= 70 \text{ years})\)

\( EF \) = Exposure frequency – resident \((= 350 \text{ days/year})\)

\( ED_c \) = Exposure duration – child \((= 6 \text{ years})\)

\( ED_r \) = Exposure duration – resident \((= 30 \text{ years})\)

\( IRS_a \) = Resident soil ingestion rate – adult \((= 100 \text{ mg/day})\)

\( IRS_c \) = Resident soil ingestion rate – child \((= 200 \text{ mg/day})\)
Using the exposure assumptions listed above, Equation (50) can be simplified as:

\[
SC_{\text{res-sol-ca-vc-ing}} = \frac{0.067}{SF} \tag{51}
\]

### 4.2.3.2 Trichloroethylene (TCE) – Soil, Ingestion

The following three steps were used to calculate a soil screening concentration benchmark reflecting exposure only via ingestion.

**Step 1.** A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the mutagenic equation provided below.

\[
SC_{\text{sol-mu-tce-ing}} = \frac{TR \times AT \times LT}{SF_{\text{kidney}} \times EF \times IFSM \times \frac{10^{-6} \text{ kg}}{\text{mg}}} \tag{52}
\]

*Where:*

- \( SC_{\text{sol-mu-tce-ing}} \) = Soil Screening Concentration, Mutagenic (mg/kg)
- \( IFSM \) = Mutagenic soil ingestion rate–resident, age adjusted \([=(489.5 \text{ mg-year})/(\text{kg-day})]\), calculated as:
  \[
  IFSM = \left( \frac{ED_{0-2} \times IRS_a \times 10}{BM_a} \right) + \left( \frac{ED_{2-6} \times IRS_a \times 3}{BM_a} \right) + \left( \frac{ED_{6-16} \times IRS_a \times 3}{BM_a} \right) + \left( \frac{ED_{16-30} \times IRS_a \times 1}{BM_a} \right)
  \]
- \( SF_{\text{kidney}} \) = Chronic oral slope factor, kidney (mg/kg-day)\(^{-1}\)
- \( TR \) = Target risk \((= 1 \times 10^{-6})\)
- \( AT \) = Averaging time – resident \((= 365 \text{ days/year})\)
- \( LT \) = Lifetime \((= 70 \text{ years})\)
- \( EF \) = Exposure frequency – resident \((= 350 \text{ days/year})\)
- \( ED_{0-2} \) = Exposure duration – resident ages 0-2 \((= 2 \text{ years})\)
- \( ED_{2-6} \) = Exposure duration – resident ages 2-6 \((= 4 \text{ years})\)
- \( ED_{6-16} \) = Exposure duration – resident ages 6-16 \((= 10 \text{ years})\)
- \( ED_{16-30} \) = Exposure duration – resident ages 16-30 \((= 14 \text{ years})\)
- \( IRS_a \) = Resident soil ingestion rate – adult \((= 100 \text{ mg/day})\)
- \( IRS_c \) = Resident soil ingestion rate – child \((= 200 \text{ mg/day})\)
- \( BM_a \) = Body mass – adult \((= 70 \text{ kg})\)
- \( BM_c \) = Body mass – child \((= 15 \text{ kg})\)

Using the exposure assumptions listed above, Equation (52) can be simplified as:

\[
SC_{\text{sol-mu-tce-ing}} = \frac{0.149}{SF_{\text{kidney}}} \tag{53}
\]
Step 2. A cancer screening concentration (SC) is calculated using the NHL and liver cancer slope factor and the cancer equation provided below.

$$SC_{sol-ca-tce-ing} = \frac{TR \times AT \times LT}{SF_{NHL\ and\ Liver} \times EF \times IFS \times 10^{-6}\ kg\ mg}$$

(54)

Where:

- $$SC_{sol-ca-tce-ing}$$ = Soil Screening Concentration, Carcinogenic (mg/kg)
- $$IFS$$ = Soil ingestion rate – resident, age adjusted $$[= (114\ mg\text{-year})/(kg\text{-day})]$$, calculated as:
  $$IFS = \left(\frac{ED_c \times IRS_c}{BM_c}\right) + \left[\frac{(ED_r - ED_c) \times IRS_a}{BM_a}\right]$$
- $$SF_{NHL\ and\ Liver}$$ = Chronic oral cancer slope factor, NHL and liver (mg/kg-day)$^{-1}$
- $$TR$$ = Target risk ($= 1 \times 10^{-6}$)
- $$AT$$ = Averaging time – resident ($= 365\ days\text{/year}$)
- $$LT$$ = Lifetime ($= 70\ years$)
- $$EF$$ = Exposure frequency – resident ($= 350\ days\text{/year}$)
- $$ED_c$$ = Exposure duration – child ($= 6\ years$)
- $$ED_r$$ = Exposure duration – resident ($= 30\ years$)
- $$IRS_a$$ = Resident soil ingestion rate – adult ($= 100\ mg\text{/day}$)
- $$IRS_c$$ = Resident soil ingestion rate – child ($= 200\ mg\text{/day}$)
- $$BM_a$$ = Body mass – adult ($= 70\ kg$)
- $$BM_c$$ = Body mass – child ($= 15\ kg$)

Using the exposure assumptions listed above, Equation (54) can be simplified as:

$$SC_{sol-ca-tce-ing} = \frac{0.64}{SF_{NHL\ and\ Liver}}$$

(55)

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations, via oral ingestion, calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{sol-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{sol-ca-ing}}\right) + \left(\frac{1}{SC_{sol-mu-ing}}\right)}$$

(56)

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative equation for calculating Step 3 results:

$$SC_{sol-ca-mu-tce-ing} = \frac{1}{1.56\ SF_{NHL\ and\ Liver} + 6.71\ SF_{kidney}}$$

(57)
4.2.4 Carcinogenic – Soil, Radionuclides

1) Oral

\[
SC_{\text{soll-ca-rad}} = \frac{TR \times t_r \times \lambda}{(1-e^{-\lambda t_r}) \times SF_s \times IFS_{r-adj} \times EF_r \times ED_r \times \left(\frac{g}{1000 \text{mg}}\right)}
\]

Where:

\[
IFS_{r-adj} = \frac{(IRS_c \times ED_c + IRS_a \times ED_{r-a})}{ED}
\]

\[
SC_{\text{soll-ca-rad}} = \text{Soil cancer screening concentration benchmark – radiochemical (pCi/g)}
\]

\[
SF_s = \text{Slope factor – soil, radiochemical – substance specific (pCi)}^{-1}
\]

\[
IFS_{r-adj} = \text{Resident soil ingestion factor (mg/day)}
\]

\[
TR = \text{Target risk (1 x 10}^{-6}\text{)}
\]

\[
t_r = \text{Time (30 years)}
\]

\[
\lambda = \text{Lamba – substance specific}
\]

\[
EF = \text{Exposure frequency – resident (350 days/year)}
\]

\[
ED = \text{Exposure duration – resident (30 years)}
\]

\[
IRS_a = \text{Soil ingestion rate – adult (100 mg/day)}
\]

\[
IRS_c = \text{Soil ingestion rate – child (200 mg/day)}
\]

\[
ED_c = \text{Exposure duration – resident child (6 years)}
\]

\[
ED_{r-a} = \text{Exposure duration – resident adult (24 years)}
\]

Using the exposure assumptions listed above, Equation (58) can be simplified as:

\[
SC_{\text{soll-ca-rad}} = 2.38 \times 10^{-11} \times \frac{\lambda}{[(1 - e^{-30\lambda}) \times SF_s]}
\]

2) External Exposure (gamma emitters)

\[
SC_{\text{ext-rad}} = \frac{TR \times t_r \times \lambda}{(1-e^{-\lambda t_r}) \times SF_{\text{ext}} \times ACF \times EF \times \left(\frac{1 \text{ year}}{365 \text{ days}}\right) \times ED \times [ET_{r-c} \times (ET_{r-a} \times GSF)]}
\]

Where:

\[
SC_{\text{ext-rad}} = \text{Screening concentration benchmark – radiochemical, external (pCi/g)}
\]

\[
SF_{\text{ext}} = \text{Slope factor – external exposure – substance specific (pCi)}^{-1}
\]

\[
TR = \text{Target risk (1 x 10}^{-6}\text{)}
\]

\[
t_r = \text{Time (30 years)}
\]

\[
\lambda = \text{Lamba – substance specific}
\]

\[
e = \text{Euler’s number (= 2.718281828)}
\]

\[
ACF = \text{Area correction factor – substance specific}
\]

\[
EF = \text{Exposure frequency – resident (350 days/year)}
\]

\[
ED = \text{Exposure duration – resident (30 years)}
\]

\[
ED_c = \text{Exposure duration – resident child (6 years)}
\]

\[
ED_{r-a} = \text{Exposure duration – resident adult (24 years)}
\]
ET_{ro} = Exposure time – resident outdoor (0.073 hr/hr)
ET_{ri} = Exposure time – resident indoor (0.684 hr/hr)
GSF_i = Gamma shielding factor – indoor (0.4), unitless
IRS_c = Soil ingestion rate – child (200 mg/day)

Using the exposure assumptions listed above, Equation (60) can be simplified as:

\[ SC_{ext-rad} = \frac{3.01 \times 10^{-6} \times \lambda}{[(1 - e^{-30\lambda}) \times SF_{ext} \times ACF]} \] (61)

### 4.3 Screening Concentration Benchmarks for the Ground Water and Drinking Water Pathways

The following equations are used to determine water ingestion screening concentration benchmarks. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA’s *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided in Section 4.3.1 (non-carcinogenic benchmarks) and Section 4.3.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 4.3.3; these equations are taken from EPA’s *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. Equations used for radionuclides are provided in Section 4.3.4.

#### 4.3.1 Non-carcinogenic – Ground Water and Drinking Water, Ingestion

\[ SC_{water-nc-ing} = \frac{THQ \times AT \times ED_c \times BM_c \times 1000 \ \mu g/mg}{EF \times ED_c \times \left(\frac{1}{RfD}\right) \times IRW_c} \] (62)

*Where:*
- \( SC_{water-nc-ing} \) = Ground Water/Drinking Water Screening Concentration, Non-Carcinogenic (\( \mu g/L \))
- \( RfD \) = Oral reference dose (in mg/kg-day)
- \( AT \) = Averaging time – resident (365 days/year)
- \( BM_c \) = Body mass – child (= 15 kg)
- \( ED_c \) = Exposure duration – child (= 6 years)
- \( EF \) = Exposure frequency – resident (= 350 days/year)
- \( IRW_c \) = Drinking water ingestion rate – resident child (= 1 L/day)
- \( THQ \) = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (62) can be simplified as:

\[ SC_{water-nc-ing} = 15642.86 \times RfD \] (63)
4.3.2 Carcinogenic – Ground Water and Drinking Water, Ingestion

\[
SC_{\text{water-ca-ing}} = \frac{TR \times AT \times LT \times 1000 \, \mu g/mg}{SF \times EF \times IFW}
\]  

(64)

Where:

- \(SC_{\text{water-ca-ing}}\) = Ground Water/Drinking Water Screening Concentration, Carcinogenic (\(\mu\)g/L)
- \(IFW\) = Drinking water ingestion rate – Resident, adjusted [\(= (1.086 \, \text{L-year}) / (\text{kg-day})\)], calculated as:
  
  \[
  = \left(\frac{ED_c \times IRW_c}{BM_c}\right) + \left(\frac{(ED_r - ED_c) \times IRW_a}{BM_a}\right)
  \]

- \(SF\) = Chronic oral slope factor (mg/kg-day)-1
- \(TR\) = Target risk (\(= 1 \times 10^{-6}\))
- \(AT\) = Averaging time – resident (\(= 365 \, \text{days/year}\))
- \(LT\) = Lifetime (\(= 70 \, \text{years}\))
- \(EF\) = Exposure frequency – resident (\(= 350 \, \text{days/year}\))
- \(ED_c\) = Exposure duration – child (\(= 6 \, \text{years}\))
- \(ED_r\) = Exposure duration – resident (\(= 30 \, \text{years}\))
- \(IRW_a\) = Drinking water ingestion rate – resident adult (\(= 2 \, \text{L/day}\))
- \(IRW_c\) = Drinking water ingestion rate – resident child (\(= 1 \, \text{L/day}\))
- \(BM_a\) = Body mass – adult (\(= 70 \, \text{kg}\))
- \(BM_c\) = Body mass – child (\(= 15 \, \text{kg}\))

Using the exposure assumptions listed above, Equation (64) can be simplified as:

\[
SC_{\text{water-ca-ing}} = \frac{0.0672}{SF}
\]  

(65)

4.3.3 Carcinogenic through a Mutagenic Mode of Action – Ground Water and Drinking Water, Ingestion

\[
SC_{\text{water-mu-ing}} = \frac{TR \times AT \times LT \times 1000 \, \mu g/mg}{SF \times EF \times IFWM}
\]  

(66)

Where:

- \(SC_{\text{water-mu-ing}}\) = Ground Water/Drinking Water Screening Concentration, Mutagenic (\(\mu\)g/L)
- \(IFWM\) = Mutagenic Drinking Water ingestion rate – resident, age adjusted [\(= (3.39 \, \text{L-year}) / (\text{kg-day})\)], calculated as:
  
  \[
  = \left(\frac{ED_{0-2} \times IRW_c \times 10}{BM_c}\right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BM_c}\right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-30} \times IRW_a \times 1}{BM_a}\right)
  \]

- \(SF\) = Chronic oral slope factor (mg/kg-day)-1
- \(TR\) = Target risk (\(= 1 \times 10^{-6}\))
- \(AT\) = Averaging time – resident (\(= 365 \, \text{days/year}\))
- \(LT\) = Lifetime (\(= 70 \, \text{years}\))
- \(EF\) = Exposure frequency – resident (\(= 350 \, \text{days/year}\))
- \(ED_{0-2}\) = Exposure duration – resident ages 0-2 (= 2 years)
- \(ED_{2-6}\) = Exposure duration – resident ages 2-6 (= 4 years)
- \(ED_{6-16}\) = Exposure duration – resident ages 6-16 (= 10 years)
Using the exposure assumptions listed above, Equation (66) can be simplified as:

\[ SC_{\text{water-mu-ing}} = \frac{0.0215}{SF} \]  

(67)

### 4.3.3.1 Vinyl Chloride – Ground Water and Drinking Water, Ingestion

\[
SC_{\text{res-water-ca-vc-ing}} = \frac{TR}{\left[ \frac{SF \times EF \times IFW \times \frac{mg}{1000 \mu g}}{AT \times LT} \right] + \left[ \frac{SF \times IRW_c \times \frac{mg}{1000 \mu g}}{BM_c} \right]} \]  

(68)

**Where:**

- \( SC_{\text{res-water-ca-vc-ing}} \) = Ground Water/Drinking Water Screening Concentration, Vinyl Chloride (µg/L)
- \( IFW \) = Drinking water ingestion rate – Resident, adjusted \([= (1.086 \text{ L-year})/(\text{kg-day})]\), calculated as:
  \[
  IFW = \frac{ED_c \times IRW_c}{BM_c} + \frac{(ED_R - ED_c) \times IRW_a}{BM_a} 
  \]

- \( SF \) = Chronic oral slope factor (mg/kg-day)\(^{-1}\)
- \( TR \) = Target risk (= 1 x 10\(^{-6}\))
- \( AT \) = Averaging time – resident (= 365 days/year)
- \( LT \) = Lifetime (= 70 years)
- \( EF \) = Exposure time – resident (= 350 days/year)
- \( ED_c \) = Exposure duration – child (= 6 years)
- \( ED_R \) = Exposure duration – resident (= 30 years)
- \( IRW_c \) = Drinking water ingestion rate – resident child (= 1 L/day)
- \( IRW_a \) = Drinking water ingestion rate – resident adult (= 2 L/day)
- \( BM_a \) = Body mass – adult (= 70 kg)
- \( BM_c \) = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (68) can be simplified as:

\[ SC_{\text{res-water-ca-vc-ing}} = \frac{0.0123}{SF} \]  

(69)

### 4.3.3.2 Trichloroethylene (TCE) – Ground Water and Drinking Water, Ingestion

The following three steps were used to calculate a drinking water screening concentration reflecting exposure only via ingestion.

**Step 1.** A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the
equation provided below.

\[
SC_{\text{water-mu-tce-ing}} = \frac{TR \times AT \times LT \times 1000}{SF_{\text{kidney}} \times EF \times IFW}
\]  

(70)

Where:

- \(SC_{\text{water-mu-tce-ing}}\) = Drinking Water Screening Concentration, Mutagenic Mode of Action (µg/L)
- \(IFW\) = Mutagenic Drinking Water ingestion rate – resident, age adjusted \([= (3.39 \text{ L-year}) / (\text{kg-day})]\), calculated as:

\[
= \left( \frac{ED_{0-2} \times IRW_c \times 10}{BM_c} \right) + \left( \frac{ED_{2-6} \times IRW_c \times 3}{BM_c} \right) + \left( \frac{ED_{6-16} \times IRW_a \times 3}{BM_a} \right) + \left( \frac{ED_{16-30} \times IRW_a \times 1}{BM_a} \right)
\]

- \(SF_{\text{kidney}}\) = Chronic oral cancer slope factor, kidney (mg/kg-day)^{-1}
- \(TR\) = Target risk \((= 1 \times 10^{-6})\)
- \(AT\) = Averaging time – resident \((= 365 \text{ days/year})\)
- \(LT\) = Lifetime \((= 70 \text{ years})\)
- \(EF\) = Exposure frequency – resident \((= 350 \text{ days/year})\)
- \(ED_{0-2}\) = Exposure duration – resident ages 0-2 \((= 2 \text{ years})\)
- \(ED_{2-6}\) = Exposure duration – resident ages 2-6 \((= 4 \text{ years})\)
- \(ED_{6-16}\) = Exposure duration – resident ages 6-16 \((= 10 \text{ years})\)
- \(ED_{16-30}\) = Exposure duration – resident ages 16-30 \((= 14 \text{ years})\)
- \(IRW_c\) = Drinking water ingestion rate – resident child \((= 1 \text{ L/day})\)
- \(IRW_a\) = Drinking water ingestion rate – resident adult \((= 2 \text{ L/day})\)
- \(BM_a\) = Body mass – adult \((= 70 \text{ kg})\)
- \(BM_c\) = Body mass – child \((= 15 \text{ kg})\)

Using the exposure assumptions listed above, Equation (70) can be simplified as:

\[
SC_{\text{water-mu-tce-ing}} = 0.0215 / SF_{\text{kidney}}
\]

(71)

Step 2. A cancer SC is calculated using the NHL and liver cancer slope factor and equation provided below.

\[
SC_{\text{water-ca-tce-ing}} = \frac{TR \times AT \times LT \times 1000 \mu\text{g/mg}}{SF_{\text{NHL and Liver}} \times EF \times IFW}
\]

(72)

Where:

- \(SC_{\text{water-ca-tce-ing}}\) = Drinking Water Screening Concentration, Carcinogenic (µg/L)
- \(IFW\) = Drinking water ingestion rate – Resident, adjusted \([= (1.086 \text{ L-year}) / (\text{kg-day})]\), calculated as:

\[
= \left( \frac{ED_c \times IRW_c}{BM_c} \right) + \left( \frac{(ED_r - ED_c) \times IRW_a}{BM_a} \right)
\]

- \(SF_{\text{NHL and liver}}\) = Chronic oral cancer slope factor, NHL and liver (mg/kg-day)^{-1}
- \(TR\) = Target risk \((= 1 \times 10^{-6})\)
- \(AT\) = Averaging time – resident \((= 365 \text{ days/year})\)
- \(LT\) = Lifetime \((= 70 \text{ years})\)
- \(EF\) = Exposure frequency – resident \((= 350 \text{ days/year})\)
Using the exposure assumptions listed above, Equation (72) can be simplified as:

\[ SC_{water-ca-tce-ing} = \frac{0.067}{SF_{NHL and liver}} \] 

(73)

**Step 3.** A cumulative result of both the oral mutagenic and oral cancer screening concentrations calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and NHL and liver cancer risk.

\[ SC_{water-ca-mu-tce-ing} = \frac{1}{\left( \frac{1}{SC_{water-ca-ing}} \right) + \left( \frac{1}{SC_{water-mu-ing}} \right)} \] 

(74)

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative to Equation 74 for calculating Step 3 results:

\[ SC_{water-ca-mu-tce-ing} = \frac{1}{14.9 SF_{NHL and Liver} + 46.5 SF_{kidney}} \] 

(75)

4.3.4 Carcinogenic – Ground Water and Drinking Water, Radionuclides

\[ SC_{c-water-rad} = \frac{TR}{EF_r \times ED_r \times SF_w \times IFW_{r-adj}} \] 

(76)

Where:

- \( IFW_{r-adj} = \frac{ED_c \times IRW_c + ED_{r-a} \times IRW_c}{ED_r} \)
- \( SC_{c-water-rad} = Drinking water screening concentration benchmark – radiochemical (pCi/L) \)
- \( SF_w = Slope factor – drinking water – substance specific (pCi)^{-1} \)
- \( TR = Target risk (1 \times 10^{-6}), \) unitless
- \( EF = Exposure frequency – resident (350 days/year) \)
- \( ED = Exposure duration – resident (30 years) \)
- \( IRW_a = Water ingestion rate – adult (2 L/day) \)
- \( IRW_c = Water ingestion rate – child (1 L/day) \)
Using the exposure assumptions listed above, Equation (76) can be simplified as:

\[ SC_{c-water-rad} = 5.29 \times 10^{-11} / SF_w \]  

(77)

### 4.4 Screening Concentration Benchmarks for the Human Food Chain Pathway

The following equations are used to determine screening concentration benchmarks for the human food chain exposure pathway. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA’s *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided in Section 4.4.1 (non-carcinogenic benchmarks) and Section 4.4.2 (carcinogenic benchmarks). Equations used for radionuclides are provided in Section 4.4.3.

#### 4.4.1 Non-carcinogenic – Human Food Chain, Fish Ingestion

\[
SC_{res-fish-nc-ing} = \frac{THQ \times AT \times ED_r \times BM_a}{EF \times ED_r \times \left( \frac{1}{RfD} \right) \times IRF \times \frac{10^{-6} \text{ kg}}{\text{mg}}} 
\]  

(78)

Where:
- \( SC_{res-fish-nc-ing} \) = Human Food Chain Screening Concentration, Fish Ingestion, Non-Carcinogenic (mg/kg)
- \( RfD \) = Oral reference dose (in mg/kg-day)
- \( AT \) = Averaging time – resident (365 days/year)
- \( BM_a \) = Body mass – adult (= 70 kg)
- \( ED_r \) = Exposure duration – resident (= 30 years)
- \( EF \) = Exposure frequency – resident (= 350 days/year)
- \( IRF \) = Fish ingestion rate (= 5.4 x 10^4 mg / day)
- \( THQ \) = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (78) can be simplified as:

\[ SC_{res-fish-nc-ing} = 1350 \times RfD \]  

(79)

#### 4.4.2 Carcinogenic – Human Food Chain, Fish Ingestion

\[
SC_{res-fish-ca-ing} = \frac{TR \times AT \times LT \times BM_a}{EF \times ED_r \times SF \times IRF \times \frac{10^{-6} \text{ kg}}{\text{mg}}} 
\]  

(80)

Where:
- \( SC_{res-fish-ca-ing} \) = Human Food Chain Screening Concentration, Fish Ingestion, Carcinogenic (mg/kg)
- \( SF \) = Chronic oral cancer slope factor (mg/kg-day)^{-1}
- \( TR \) = Target risk (= 1 x 10^{-6})
Using the exposure assumptions listed above, Equation (80) can be simplified as:

\[
SC_{\text{res-fish-ca-ing}} = \frac{0.00315}{SF} \quad (81)
\]

### 4.4.3 Carcinogenic – Human Food Chain, Fish Ingestion, Radionuclides

\[
SC_{\text{c-fish-rad}} = \frac{TR}{EF \times ED \times SF_f \times IRF} \times \frac{g}{1000 \text{mg}} \quad (82)
\]

Where:
- \(SC_{\text{c-fish-rad}}\) = Human Food Chain Screening Concentration, Fish Ingestion – Radiochemical, Carcinogenic (pCi/g)
- \(SF_f\) = Slope factor – drinking water – substance specific (pCi)⁻¹
- \(TR\) = Target risk (1 x 10⁻⁶), unitless
- \(EF\) = Exposure frequency – resident (350 days/year)
- \(ED\) = Exposure duration – resident (30 years)
- \(ED_c\) = Exposure duration – resident child (6 years)
- \(ED_{ra}\) = Exposure duration – resident adult (24 years)
- \(IRF\) = Fish ingestion rate (= 5.4 x 10⁴ mg / day)

Using the exposure assumptions listed above, Equation (82) can be simplified as:

\[
SC_{\text{c-fish-rad}} = 1.76 \times 10^{-12} / SF_f \quad (83)
\]
5.0 SCDM DATA REPORTING and APPENDICES

5.1 Data Reporting

Data are collected from the references identified in Section 2 of this document. The data are collected exactly as provided in the references and compiled into a SCDM data management tool. Once in the tool, converted values are generated to reflect the SCDM standard units for use in calculations, while the original values remain unchanged for transparency. Collected data and calculated results are maintained in the tool and are not rounded, truncated or otherwise adjusted except for purposes of reporting in SCDM Appendices A, BI and BII.

The following rules are applied for purposes of reporting SCDM data in Appendices A, BI and BII:

- Substance characterization data and data that serve as inputs to benchmark and factor value formulas are truncated and reported to two significant figures.
- Screening concentration benchmarks are truncated to the number of significant figures contained in the data input variable (i.e., RfD,RFC, IUR, or cancer slope factor) used to determine each benchmark. For example, a screening concentration benchmark determined using a cancer slope factor of 2.81E-8, will be reported to three significant figures.
- Factor values will be reported to the number of significant figures needed to support decision making as described at 40 CFR Part 300 Appendix A and 55 FR 51583.

5.2 SCDM Appendices

Appendix A of SCDM contains selected data, HRS factor values and benchmarks for each hazardous substance in SCDM (the “SCDM page reports”). Information is provided in a two-page report for each substance. Data selected for SCDM are on the first page; factor values and benchmarks are on the second page.

Figure 1 presents an example of the header that appears on the Appendix A report. The header contains the date the report was created, the substance name and synonym, and the Chemical Abstract Survey Registration Number (CAS Number) for the substance.

For each substance, the first page contains all of the selected chemical data, the data units, and an acronym describing the reference source of the information. Data are divided into six functional groups: toxicity, persistence, physical characteristics, mobility, bioaccumulation and other data. The “SCDM Data Version” date in the upper left-hand corner indicates the date of data collection; the “Publication Date” indicates the date the report was generated and posted on the SCDM website at http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm.

The toxicity section (Figure 2) contains the acute, chronic, and carcinogenicity data that were compiled using the methodology described in Sections 2.2 and 2.6, and used to derive toxicity and ecotoxicity factor values.
### TOXICITY

<table>
<thead>
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<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral RfD:</td>
<td>6.0E-2</td>
<td>mg/kg/day</td>
<td>IRIS</td>
</tr>
<tr>
<td>Inhal RfD:</td>
<td></td>
<td>mg/kg/day</td>
<td></td>
</tr>
<tr>
<td>RfC:</td>
<td></td>
<td>mg/m^3</td>
<td></td>
</tr>
<tr>
<td>Oral Slope:</td>
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</tr>
<tr>
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<td></td>
</tr>
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<td>IUR:</td>
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<td>(mg/kg/day)^-1</td>
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<td>Oral ED10:</td>
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</tr>
<tr>
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<td></td>
<td></td>
</tr>
<tr>
<td>Oral ED10 Wgt:</td>
<td></td>
<td>mg/kg/day</td>
<td></td>
</tr>
<tr>
<td>Inhal ED10 Wgt:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oral LD50:</td>
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<td>mg/kg</td>
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</tr>
<tr>
<td>Dermal LD50:</td>
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<tr>
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<tr>
<td>Dust Inhal LC50:</td>
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<td>mg/L</td>
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</tr>
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<tr>
<td>Salt CMC:</td>
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<td>μg/L</td>
<td></td>
</tr>
<tr>
<td>CHRONIC</td>
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<td></td>
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<td>μg/L</td>
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<tr>
<td>Salt Ecol LC50:</td>
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<td></td>
<td>ECOTOX</td>
</tr>
</tbody>
</table>

**Figure 2. Toxicity Section**

The top half of this section contains the data used to determine the HTF value: reference dose (oral and inhalation), cancer slope factor (oral and inhalation unit risk [IUR]), ED_{10} (oral and inhalation), LD_{50} (oral and dermal) and LC_{50} (gas and dust inhalation). The bottom half of this section contains the data used to determine an ecotoxicity factor value: acute and chronic water quality criteria, CMC and CCC, for fresh and salt water as well as fresh and salt water LC_{50} values. Blank entries indicate that no value was found using the procedures and references specified.

The persistence section (Figure 3) contains the surface water persistence data compiled using the methodology described in Section 2.4. Surface water persistence factors can also be determined using the logarithm of the n-octanol/water partition coefficient (Log K_{ow} or Log P, Section 2.3) if, as specified in the HRS, this gives a higher factor value than the half-lives (or a default, if applicable).
### PERSISTENCE

<table>
<thead>
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<td>days</td>
<td>THOMAS</td>
</tr>
<tr>
<td>Volatility:</td>
<td>2.5E+0</td>
<td>days</td>
<td>HEDR</td>
</tr>
<tr>
<td>Photolysis:</td>
<td>1.0E+2</td>
<td>days</td>
<td>HEDR</td>
</tr>
<tr>
<td>Radio:</td>
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<table>
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<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
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</thead>
<tbody>
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<td></td>
<td></td>
</tr>
<tr>
<td>Hydrolysis:</td>
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<td>days</td>
<td>THOMAS</td>
</tr>
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<td>days</td>
<td>HEDR</td>
</tr>
<tr>
<td>Photolysis:</td>
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<td>HEDR</td>
</tr>
<tr>
<td>Radio:</td>
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</tr>
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</table>

**Log Kow:** 3.9E+0  EPI

---

**Figure 3. Persistence Section**

The physical characteristics section (Figure 4) contains logical “yes/no” flags that classify the substance. The “metal contain” flag indicates that the hazardous substance is a metal or metalloid and is used to determine ground water mobility and surface water persistence factors. The “organic” and “inorganic” flags are used to determine ground water mobility and bioaccumulation. The “radionuclide” flag is used to determine the HTF, the ecosystem toxicity factor and the surface water persistence factor. The radioactive element flag (“rad. element”) is used to determine whether or not the HRS factors and benchmarks (second page) are printed. The gas and particulate flags are used to determine mobility and likelihood of release for the air pathway. MW is used to determine volatilization half-life.

### PHYSICAL CHARACTERISTICS

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<tr>
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<td>Rad. Element:</td>
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<td>Density:</td>
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</table>

**Figure 4. Physical Characteristics Section**

The mobility section (Figure 5) contains the air and ground water mobility data compiled using the methodology described in Section 2.3. Vapor pressure and HLC are used to determine gas migration potential and gas mobility factors. HLC is also used to calculate the volatilization half-life. Water solubility and the soil/water distribution coefficient are used to determine the ground water mobility factor. Substance-specific water solubility is used for nonmetal and non-metalloid substances, whereas for metal-containing substances, the solubility value is the geometric mean of the available water solubilities for inorganic compounds containing the hazardous substance.
### MOBILITY

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</table>

**Figure 5. Mobility Section**

The bioaccumulation section (Figure 6) contains the human food chain and environmental bioaccumulation potential factor data compiled using the methodology described in Section 2.5. BCFs are collected for fresh and saltwater for the human food chain and environmental threats. Log K_{ow} or water solubility is used to establish bioaccumulation potential when a BCF is not available.

### BIOACCUMULATION

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<tr>
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<tr>
<td>Salt BCF</td>
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</tr>
<tr>
<td>Log Kow</td>
<td>3.9E+0</td>
<td>EPI</td>
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<tr>
<td>Water Solub</td>
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<td>PHYSPROP</td>
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<tr>
<td>Geo Mean Sol</td>
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</table>

**Figure 6. Bioaccumulation Section**

The section labeled “other data” (Figure 7) contains values for melting points and boiling points (°C) along with the associated vapor pressure (Torr), if applicable. The chemical formula is also listed here.

### OTHER DATA

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**Figure 7. Other Data**

The class information section (Figure 8) lists parent substances for three data substitution classes: toxicity, ground water mobility and other data. The toxicity class includes all toxicity and benchmark data used to determine human or ecotoxicity factor values. The ground water mobility class includes water solubility, K_{d}, and geometric mean water solubility. The “other” class includes hydrolysis, biodegradation, photolysis and volatilization half-lives, as well as BCFs and Log K_{ow}. This section may also list other class-parent chemical substitutions for specific data elements.
Currently, only two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for the ground water mobility class with the elemental metal as the class parent. Radioactive isotopes may inherit data from their primary radioactive element for the ground water mobility and “other” classes.

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The second page for each substance is divided into top and bottom sections that contain factor values (Figure 9) and benchmarks (Figure 10) required by the HRS. SCDM determines factor values using HRS methodologies from selected data on the first page of the SCDM page report. The factor values are presented by exposure pathway: air, ground water, soil and surface water. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. The toxicity factor value represents human toxicity and is the same for all pathways. The air pathway gas migration factor value is used to determine likelihood of release. The surface water environmental toxicity factor values are based on fresh and saltwater ecosystem toxicity data, and the surface water persistence factor values are based on BCFs for all aquatic species. The surface water human food chain factor values are based on human toxicity and BCFs for only those aquatic species consumed by humans. For radioactive substances, human toxicity, ecosystem toxicity and surface water persistence factor values are determined as specified in Section 7 of the HRS.
### ASSIGNED FACTOR VALUES

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### SURFACE WATER PATHWAY

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**Figure 9. Assigned Factor Values Section**

The benchmarks (Figure 10), like the factor values, are presented by pathway: air, ground water, soil exposure, and surface water. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. For HRS scoring, actual sample contaminant concentrations for a particular medium are compared to these benchmark concentrations to determine if the target will be scored as subject to Level I or Level II concentrations.
## BENCHMARKS

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## SURFACE WATER PATHWAY

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**Figure 10. Benchmarks Section**

Appendix B is divided into two sections, Appendix B-I and B-II. Appendix B-I contains all of the factor values by exposure pathway. Factor values for non-radionuclide substances are listed first and are followed by a listing of factor values for radionuclides. Appendix B-II presents all the screening concentration benchmarks by exposure pathway. Benchmarks are provided for the drinking water/groundwater and surface water exposure pathways, followed by the air and soil exposure pathways. Benchmarks for non-radionuclide substances are provided first, followed by benchmarks for the radionuclides. Appendix C contains a cross-reference index of hazardous substance names, synonyms and CAS Numbers for substances in SCDM.
6.0 REFERENCES

- U.S. EPA, Superfund Chemical Data Matrix (SCDM). 
  http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm


• U.S. EPA. 2012. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/ecotox

• EPI Suite™. Developed by the U.S. Environmental Protection Agency’s Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm


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*Note: All values are in ng/L except for Karst and Non-Karst mobility, which are in ng/L/m²/y.*
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<th>CAS Number</th>
<th>Toxicity</th>
<th>Ground Water Mobility</th>
<th>Hazardous Substance Factor Values</th>
<th>Ecotoxicity</th>
<th>Air Gas Migration/Mobility</th>
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* Value was modified since the January 2014 publication of SCDM. See Change Control documentation for details (http://www.epa.gov/superfund/sites/npl/hrsres/tools/changecontrol.pdf)
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<th>Bioaccumulation</th>
<th>Ecotoxicity</th>
<th>Air Gas Migration/Mobility</th>
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<th>Persistence</th>
<th>Bioaccumulation</th>
<th>Ecotoxicity</th>
<th>Air Gas Migration/Mobility</th>
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### HAZARD RANKING SYSTEM

**Hazardous Substance Factor Values**

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