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

[July 2020]

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 51532; 82 FR 2760) to evaluate potential National Priorities List (NPL) sites. The HRS assigns factor values including those for toxicity, gas and vapor migration potential, gas and ground water mobility, surface water persistence, subsurface intrusion (SSI) degradation, 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 current factor values and benchmarks published in the SCDM Web Query and changes noted in the SCDM Change Control and Errata Sheet (described below) supersede any previous values provided by SCDM. These 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 Web Query) describes how SCDM data, HRS factor values, and screening concentration benchmarks are presented.

Data inputs, factor values and benchmarks are listed, by substance and Chemical Abstracts Survey Registry Number (CASRN), in the SCDM Web Query (http://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm-query).
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 2.8 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.

The references listed throughout Section 2.2 of this methodology document were last accessed during August – November 2012, in preparation for a comprehensive update to SCDM, which was published in January 2014. Any changes or additions since then are noted in the SCDM Change Control and Errata Sheet (available at: https://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm).

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 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. There are also cases where references or reference hierarchies other than those described in Section 2.2 are used. These special cases are described in Sections 2.1.1 through 2.1.6 below.

2.1.1 Generic Values

SCDM contains generic values for the following classes of compounds:

- 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.

- Chromium (all 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 RfD, reference concentration (RfC), SF and inhalation unit risk (IUR) values from chromium VI to total chromium.

- Endosulfans – SCDM contains data for an endosulfan mixture and two endosulfan isomers (endosulfan I and endosulfan II). The RfD and distribution coefficient data are collected for endosulfan and applied to the endosulfan mixture and its isomers. SCDM contains a vapor pressure and Henry’s Law Constant for each isomer.
• Polyaromatic hydrocarbons (PAHs) – SCDM contains SF and IUR values for benzo(a)pyrene. When a SF and/or IUR are not available for similar PAHs listed in SCDM, SCDM applies relative potency factors (RPFs) to determine values for these substances. PAH-specific RPFs are obtained from EPA’s Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089), July 1993. RPFs are not used to generate non-cancer values for PAHs (e.g., RfD or RfC).

• Polychlorinated dibenzo-dioxins and furans – SCDM contains SF, IUR, RfD, and RfC values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). When a SF, IUR, RfD and/or RfC 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.

• 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.

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

- 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 K_d value of 1,000, as stated in the HRS.

- Bromodichloromethane – SCDM assigns an MCL to bromodichloromethane based on the MCL listed for total trihalomethanes (including bromodichloromethane, bromoform, dibromochloromethane, and chloroform). Concentrations of trihalomethanes can be added to determine if drinking water is at or above the MCL.

- 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.

- Chloroform – SCDM assigns an MCL to chloroform based on the MCL listed for total trihalomethanes (including bromodichloromethane, bromoform, dibromochloromethane, and chloroform). Concentrations of trihalomethanes can be added to determine if drinking water is at or above the MCL.

- 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 80 kg body mass, 30 years exposure, and 2.5 L/day ingestion.

- 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)].

- Mercuric chloride – SCDM assigns an RfC for mercuric chloride using the following molecular weight conversion of the RfC assigned to mercury: RfC (mercuric chloride) = RfC (elemental mercury) x [molecular weight (mercuric chloride) / molecular weight (elemental mercury)]. SCDM also assigns an MCL for mercuric chloride using the following molecular weight conversion of the MCL assigned to mercury: MCL (mercuric chloride) = MCL (elemental mercury) x [molecular weight (mercuric chloride) / molecular weight (elemental mercury)].

- Radium 226 (+D) and Radium 228 (+D) – SCDM assigns an MCL to Radium-226 and Radium-228 based on the combined MCL listed for Radium-226 and Radium-228. Concentrations of Radium-226 and Radium-228 can be added to determine if drinking water is at or above the combined MCL.

- 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)].

- Vanadium – SCDM assigns an RfD for vanadium using the following molecular weight conversion of the RfD available for vanadium pentoxide: RfD (vanadium) = RfD (vanadium pentoxide) x [molecular weight (vanadium) / molecular weight (vanadium pentoxide)].

2.1.5 Substances with Unique Reference Hierarchy Selections

- Uranium – An ATSDR intermediate minimal risk level for “uranium, soluble salts” is selected for an RfD, in accordance with the December 21, 2016 U.S. EPA memorandum Considering a Noncancer Oral Reference.
2.1.6 Substances with Unique Identifiers

There is no CASRN specific to uranium 238 (+D) (radionuclide). Therefore, the EPA identification number of E1734789 is used in its place. Information regarding EPA identification numbers may be found from the EPA Substance Registry Service (SRS, accessible online at http://ofmpub.epa.gov/sor_internet/registry/substreg/home/overview/home.do).

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:

- U.S. EPA Preliminary Remediation Goals (PRGs) for Radionuclides. Office of Superfund Remediation and Technology Innovation (OSRTI). http://epa-prgs.ornl.gov/radionuclides/download.html. Primary PRG source documents include:


Accompanying area correction factors (ACFs) and decay constants (lambda) are also collected from the PRG source cited above.

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


The Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs). http://www.atsdr.cdc.gov/mrls/mrllist.asp (non-cancer data only)

The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values, Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp.


ATSDR provides MRLs for acute (1 – 14 days), intermediate (>14 – 364 days), and chronic (365 days and longer) exposure durations. SCDM does not use MRLs that are based on acute exposure. Similarly, PPRTV, PPRTV Appendix, and HEAST provide RfD and RfC values (or PPRTV Appendix screening levels) for chronic and subchronic exposure durations. During SCDM data collection, preference is given to values that are based on chronic exposure. SCDM may use intermediate MRLs or subchronic RfDs or RfCs only if no chronic value is available from any reference in the above hierarchy.

Where intermediate MRLs are used in SCDM, the reference provided in the SCDM Web Query report is “ATSDR-Int.” Where subchronic RfDs or RfCs from PPRTV or HEAST, or subchronic PPRTV Appendix screening levels, are used in SCDM, the reference provided in the SCDM Web Query report is “PPRTV-Sub,” “HEAST-Sub” or “PPRTV_APP-Sub.”

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


The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values, Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp.

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). Where a WOE classification is available without a corresponding cancer risk, the available WOE will still be collected. If a WOE classification is available for one route (oral or inhalation) but not the other, it is applied to both routes unless reference information indicates a route restriction. 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, 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 ED₁₀ and Weight-of-Evidence – Oral, Inhalation

When a cancer SF with WOE is not available, SCDM uses ED₁₀ oral and inhalation values to calculate cancer SF (see Section 3.1 of this methodology document). SCDM does not assign ED₁₀ values to radionuclides. For all other substances, SCDM uses data from the following references, listed in order of preference for oral and inhalation ED₁₀ and associated WOEs:


ED₁₀ 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. Values that are included in EPA_ED10 are provided as potency factors; the reciprocal of these potency factors are used as ED₁₀ values in SCDM.
2.3 Mobility/Volatility Information

Vapor pressures and Henry’s Law Constants are used to determine the gas migration potential, gas mobility potential, and whether a substance is treated as a gas and/or particulate for the air migration pathway. They are also used to determine the vapor migration potential and whether a substance is considered volatile for the SSI component. 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—this approach is applied for the purposes of determining whether a substance qualifies as a gas and/or particulate for the air migration pathway and assigning a vapor pressure value in evaluating the air migration pathway gas migration potential factor value.

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:

  13: 978-1439855119.


- Perry’s Chemical Engineers’ Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W.,

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 3.8 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 Kd according to HRS Section 3.2.1.2 (Mobility) and the
relationship of Kd = Koc x fS (see Section 3.5 of this methodology document), where fS is the sorbent content
(fraction of clays plus organic carbon) and Koc 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). http://www.epa.gov/tsca-screening-
tools/epi-suite-estimation-program-interface.


  Emergency and Remedial Response, Washington, DC. NTIS PB96-963502.

- Estimated as described in Section 3.5 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 3.5 (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.

The exceptions to this hierarchy are the $K_{OC}$ values for ionizable organic substances that are included in Table 42 in Part 5 of the Soil Screening Guidance: Technical Background Document cited above (derivation of these values is provided in Appendix L of the same document). For these substances, the $K_{OC}$ is assigned based on values listed for pH 6.8 in Table 42 of that document instead of values available in the above hierarchy.

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 3.5 of this methodology document).

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

### 2.4 Persistence/Degradation Information

The evaluation of persistence for non-radionuclides in the surface water migration pathway is based primarily on hydrolysis, biodegradation, photolysis and volatilization half-lives of hazardous substances in surface water and secondarily on the sorption of the hazardous substances to sediments; for radionuclides the evaluation is based on volatilization and radioactive half-lives. Persistence information is used to determine the surface water persistence factor value.

The evaluation of degradation for the subsurface intrusion component is based on the SsI hydrolysis and SsI biodegradation half-lives of hazardous substances in the subsurface for non-radionuclides, and on radioactive half-life for radionuclides. Degradation information is used with other site-specific information to determine site-specific SsI degradation factor values. These SsI degradation factor values are based on site conditions and, therefore, not included in SCDM.
2.4.1 Surface Water 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:


- **EPI Suite™** (estimated values, HYDROWIN hydrolysis half-life estimates and BioHCwin biodegradation half-life estimates; does not apply to photolysis values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

For collection of hydrolysis and biodegradation half-lives, SCDM uses aqueous half-life values. Only aerobic biodegradation half-lives are collected. If values are obtained from HEDR, SCDM uses only values listed as “first-order.” If multiple values are provided from a given reference, the highest value is used. For photolysis half-life values collected from HEDR and HSDB, both direct photolysis and indirect photolysis (or photooxidation) half-lives are collected, if available. If only a direct or indirect photolysis value is available, that value is used as the SCDM final photolysis half-life. If both direct and indirect photolysis values are available from a given reference, a final photolysis half-life is calculated as described in Section 3.2 of this methodology document. For photolysis half-lives collected from HSDB, if the photolysis mechanism (direct or indirect) is unspecified, the value is used to determine a final photolysis half-life only if no direct and/or indirect photolysis half-life is available.

If the reference from which half-lives are collected contains half-lives that apply specifically and separately to rivers and lakes, the values are used for the specified water body in SCDM. If different values for each water body type are not available, the half-life value collected is applied to both rivers and lakes.

2.4.2 SsI Hydrolysis and SsI Biodegradation Half-Lives

SCDM assigns SsI hydrolysis and SsI biodegradation half-lives only to non-radionuclide substances that qualify as SsI volatile (see Section 2.8 of this methodology document regarding determination of SsI volatility). SsI hydrolysis and SsI biodegradation half-lives are obtained from the same reference hierarchy used in Section 2.4.1 of this methodology document.

SCDM assigns SsI hydrolysis the same values collected for lakes as described in Section 2.4.1 of this methodology document.

For collection of SsI biodegradation half-lives, SCDM employs the following procedure:

- Values are considered for the following four matrix/mechanism scenarios: aqueous/aerobic, aqueous/anaerobic, soil/aerobic, and soil/anaerobic.

- If multiple half-lives are available for a specific matrix/mechanism in a given reference, the longest value will be selected for that matrix/mechanism for further consideration. This will result in up to four matrix/mechanism values from the reference for further consideration (the longest aqueous/aerobic half-life,
longest aqueous/anaerobic half-life, longest soil/aerobic half-life, and longest soil/anaerobic half-lives available in the reference).

- Of the possible four matrix/mechanism values selected in the step above from a given reference for further consideration, the shortest half-life will be collected as the SsI biodegradation half-life.

- SsI biodegradation half-life values will be collected from the most preferred reference from which any biodegradation data are available (i.e., an available half-life for one matrix/mechanism scenario from a more preferred reference will not be compared to a half-life value for another matrix/mechanism from a less preferred reference).

2.4.3 Volatilization Half-Lives

SCDM estimates volatilization half-lives for organic substances in both rivers and lakes, using the equations and procedures described in Section 3.3 of this methodology document. Volatilization half-lives are not collected or estimated for inorganic substances.

2.4.4 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_{OW} 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.
http://www.epa.gov/chemical-research/ecotoxicology-database.


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 or data reported as approximations are considered non definitive and are not used in SCDM. SCDM uses BCF values derived from wet weight data. Values derived from dry weight data are not selected. When BCF values are reported as a range, the upper limit of the range is selected.

**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>Aquatic Organism</th>
<th>Aquatic Organism</th>
<th>Aquatic Organism</th>
<th>Aquatic Organism</th>
<th>Aquatic Organism</th>
</tr>
</thead>
<tbody>
<tr>
<td>American or Virginia oyster</td>
<td>Common carp</td>
<td>Green sunfish</td>
<td>Oyster</td>
<td>Pacific oyster</td>
</tr>
<tr>
<td>Atlantic salmon</td>
<td>Common limpet, flither</td>
<td>Gudgeon</td>
<td>Pacific oyster</td>
<td>Pinfish</td>
</tr>
<tr>
<td>Bay scallop</td>
<td>Common mud crab</td>
<td>Japanese eel</td>
<td>Pink salmon</td>
<td>Pink salmon</td>
</tr>
<tr>
<td>Bay shrimp, sand shrimp</td>
<td>Common or edible winkle</td>
<td>Japanese littleneck clam</td>
<td>Pink shrimp, common</td>
<td>Pink shrimp, common</td>
</tr>
<tr>
<td>Bent-nosed clam</td>
<td>Common rangia or clam</td>
<td>Japanese whiting</td>
<td>prawn</td>
<td>prawn</td>
</tr>
<tr>
<td>Bivalve</td>
<td>Common shrimp, sand shrimp</td>
<td>Lake trout, siscowet</td>
<td>Porcelain crab</td>
<td>Porcelain crab</td>
</tr>
<tr>
<td>Bivalve/clam/mussel class</td>
<td>Crab</td>
<td>Lake whitefish</td>
<td>Porgy</td>
<td>Porgy</td>
</tr>
<tr>
<td>Black abalone</td>
<td>Crayfish</td>
<td>Lamp mussel</td>
<td>Rainbow trout</td>
<td>Rainbow trout</td>
</tr>
<tr>
<td>Black bullhead</td>
<td>Daggerblade grass shrimp</td>
<td>Large mouth bass</td>
<td>Red abalone</td>
<td>Red abalone</td>
</tr>
<tr>
<td>Blue crab</td>
<td>Dog whelk, Atlantic</td>
<td>Leopard frog</td>
<td>Red sea bream</td>
<td>Red sea bream</td>
</tr>
<tr>
<td>Bluegill</td>
<td>dogwinkle</td>
<td>Limpet</td>
<td>Red swamp crayfish</td>
<td>Red swamp crayfish</td>
</tr>
<tr>
<td>Bony fishes</td>
<td>Dungeness or edible crab</td>
<td>Longnose killifish</td>
<td>River limpet</td>
<td>River limpet</td>
</tr>
<tr>
<td>Brook silverside</td>
<td>Eastern lamp mussel</td>
<td>Mangrove oyster</td>
<td>Rough periwinkle</td>
<td>Rough periwinkle</td>
</tr>
<tr>
<td>Brook trout</td>
<td>Edible or rock crab</td>
<td>Marine bivalve</td>
<td>Scallop</td>
<td>Scallop</td>
</tr>
<tr>
<td>Brown shrimp</td>
<td>European lobster</td>
<td>Marsh grass shrimp</td>
<td>Short-necked clam</td>
<td>Short-necked clam</td>
</tr>
<tr>
<td>Bullfrog</td>
<td>Filefish</td>
<td>Marsh snail</td>
<td>Slipper limpet</td>
<td>Slipper limpet</td>
</tr>
<tr>
<td>Carp</td>
<td>Flat, native European oyster</td>
<td>Mediterranean mussel</td>
<td>Snail</td>
<td>Snail</td>
</tr>
<tr>
<td>Catfish</td>
<td>Freshwater crab</td>
<td>Minnow, carp family</td>
<td>Sole order</td>
<td>Sole order</td>
</tr>
<tr>
<td>Channel catfish</td>
<td>Freshwater mussel</td>
<td>Mud crab</td>
<td>Spot</td>
<td>Spot</td>
</tr>
<tr>
<td>Chinook salmon</td>
<td>Fresh-water mussel</td>
<td>Mummichog</td>
<td>Starrry flounder</td>
<td>Starrry flounder</td>
</tr>
<tr>
<td>Clam</td>
<td>Gizzard shad</td>
<td>Mussel</td>
<td>Striped mullet</td>
<td>Striped mullet</td>
</tr>
<tr>
<td>Cockle</td>
<td>Golden shiner</td>
<td>Mussel family</td>
<td>Swan mussel</td>
<td>Swan mussel</td>
</tr>
<tr>
<td>Coho salmon, silver salmon</td>
<td>Grass shrimp, freshwater</td>
<td>Mussel, eastern elliptio</td>
<td>Taiwan abalone</td>
<td>Taiwan abalone</td>
</tr>
<tr>
<td>Common bay mussel, blue mussel</td>
<td>prawn</td>
<td>Netted dog whelk</td>
<td>Two spot goby</td>
<td>Two spot goby</td>
</tr>
<tr>
<td></td>
<td>Great scallop</td>
<td>Northern krill</td>
<td>Unionid clam</td>
<td>Unionid clam</td>
</tr>
<tr>
<td></td>
<td>Green mussel</td>
<td>Northern pink shrimp</td>
<td>Wedge clam</td>
<td>Wedge clam</td>
</tr>
<tr>
<td></td>
<td>Green or European shore crab</td>
<td>Opossum shrimp</td>
<td>White mullet</td>
<td>White mullet</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Whitefish</td>
<td>Whitefish</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Zebra mussel</td>
<td>Zebra 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.

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 (acknowledged in HRS Section 1.1 [Definitions] in the 2017 HRS SS1 Addition, 82 FR 2760). 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 LC$_{50}$ - Freshwater, Saltwater

SCDM obtains LC$_{50}$ data from the ECOTOX database for both freshwater and saltwater.


SCDM uses the lowest acute LC$_{50}$ 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, LC$_{50}$ values are not entered into SCDM. SCDM does not use ecological LC$_{50}$ results that are qualified as labile, dissolved, or unionized. Data that are reported in the references as less than or greater than a particular value or data reported as approximations are considered non definitive and are not used in SCDM. When LC$_{50}$ values are presented as a range, the lowest value is collected.
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:


(Although NPDWS is the primary source of MCLs, MCLs for beta-emitting radionuclides are collected from the Soil Screening Guidance document where the NPDWS values in units of millirem/year are converted to pCi/L.)

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). Where available, both MCLs and MCLGs are collected for non-radionuclide substances; only MCL values are collected for radionuclide substances.

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)

Uranium Mill Tailings Radiation Control Act (UMTRCA) standards are used to establish Level I concentrations. Targets exposed to concentrations at or above UMTRCA standards are scored as Level I targets. SCDM extracts UMTRCA data directly from 40 CFR Part 192 (Uranium Mill Tailings Radiation Control Act Standards).

http://www.ecfr.gov/cgi-bin/text-index?SID=2315f900f6e83727c94e050ced329934&mc=true&node=pt40.25.192&rgn=div5#se40.25.192_102.

2.8 Physical Properties and Other Data

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point and melting point. SCDM also includes several other parameters used to classify substances based on physical properties and other aspects as described below:

Metal-Containing Substances ("Metal Contain"): “Yes” indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. “No” 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.

Organic Substances ("Organic"): “Yes” indicates that the substance is organic, and “No” indicates an inorganic substance. This flag is used to determine factor values for ground water mobility and bioaccumulation potential. These flags influence the SCDM calculation of Kd values.

Air Pathway Gas: “Yes” indicates that the vapor pressure for the substance is greater than or equal to 10^{-9} torr, and that the substance may be evaluated as a gas in the HRS air migration pathway under HRS Section 6.1.2.1 (Gas potential to release). “No” indicates that the vapor pressure for the substance does not meet this criterion, or that a vapor pressure value is not available. For organic substances, if a vapor pressure is not available, for the purpose of determining the Air Pathway Gas value, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atm is <25°C, the substance is assumed to be a gas at 25°C and a value of “Yes” is assigned. For decay chain (+D) radionuclide substances, available vapor pressure and boiling point information for the non-decay chain radionuclide or elemental counterpart are considered in assigning this flag.

Air Pathway Particulate: “Yes” indicates that the vapor pressure for the substance is less than or equal to 10^{-1} torr, and that the substance may be evaluated as a particulate in the HRS air migration pathway under HRS Section 6.1.2.2 (Particulate potential to release). “No” indicates that the vapor pressure for the substance does not meet this criterion. For organic substances, if a vapor pressure is not available, for the purpose of determining the Air Pathway Particulate value, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atm is ≥25°C, the substance is assumed to be a particulate at 25°C and a value of
“Yes” is assigned. If no vapor pressure/boiling point information is available, then the substance is assigned a “Yes” for the air pathway particulate flag. For decay chain (+D) radionuclide substances, available vapor pressure and boiling point information for the non-decay chain radionuclide or elemental counterpart are considered in assigning this flag.

**SsI Volatile:** “Yes” indicates that the substance meets the following SsI component criteria for volatility: vapor pressure greater than or equal to one torr or an HLC greater than or equal to $10^{-5}$ atm-m$^3$/mol. “No” indicates that neither the HLC nor the vapor pressure meet these criteria, or that neither a HLC nor a vapor pressure is available for the substance. This flag is used to indicate a substance’s eligibility in several aspects of the SsI component evaluation; this flag also determines whether some SsI-related values are populated, e.g., vapor migration potential, SsI hydrolysis, SsI biodegradation, and SsI overall half-lives. [Note that, as previously described, substitute chemical data are generally not applied to radioactive isotope decay chains (“+D” substances); therefore these substances do not have HLC or vapor pressure data listed in SCDM. For guidance on SsI component scoring of decay chain substances, please contact EPA Headquarters.]

**Radioactive Isotope (“Radionuclide”):** “Yes” indicates that the substance is a specific radioactive isotope, and “No” 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”):** “Yes” indicates that the substance is a radioactive element, and “No” indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag determines which HRS factor values and benchmarks will be included in the SCDM Web Query.

**Mutagen:** “Yes” indicates that the substance is known to be carcinogenic by a mutagenic mode of action. This flag affects the selection of equations for calculating screening concentration benchmarks. Information on substances considered carcinogenic by a mutagenic mode of action is obtained from the following sources:

**K_{OC} Equation:** For organic substances, this flag determines which equation will be used to calculate a K_{OC} from a K_{OW} when a K_{OC} is not available in references. See Section 3.5 of this methodology document describing the specific equations. A value of 1 indicates the first equation is used, applying to most organic substances. A value of 2 indicates the second equation is used, applying to some volatile organic compounds, chlorinated benzenes, and certain chlorinated pesticides as specified in the Soil Screening Guidance Technical Background Document (EPA, 1996). This field is populated as follows:

- If the substance is listed in the Soil Screening Guidance Technical Background Document Table 39, SCDM assigns the K_{OC} Equation value from that table.
- If the substance is not in Soil Screening Guidance Technical Background Document Table 39 and is a chlorobenzene (a benzene with one or more chlorines and no other functional groups), SCDM assigns a K_{OC} Equation value of 2.
- If neither of the above applies, and the substance is listed as a volatile organic compound in Contract Laboratory Program analytical methodology at the time of the Soil Screening Guidance document (OLM03.1), SCDM assigns a K_{OC} Equation value of 2.
- If none of the above applies, SCDM assigns a K_{OC} Equation value of 1.

### 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:


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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 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 (SF\textsubscript{oral} and SF\textsubscript{inhal}) as shown below. These ED10-determined slope factors are used to determine human toxicity factor values; they are not used in determining screening concentration benchmarks.

\[
\text{SF}_{\text{oral}} = \frac{1}{(6 \times \text{ED10}_{\text{oral}})}
\]  
\(3\)

\[
\text{SF}_{\text{inhal}} = \frac{1}{(6 \times \text{ED10}_{\text{inhal}})}
\]  
\(4\)

3.2 Photolysis Half-Life

In instances where both direct and indirect photolysis half-lives are available, SCDM combines the two to calculate a final photolysis half-life for lakes (Equation 5) or rivers (Equation 6) as follows:

\[
PHALFL_{\text{FINAL}} = \frac{1}{1 \div \text{PHALFL}_{\text{D}} + 1 \div \text{PHALFL}_{\text{I}}}
\]  
\(5\)

Where:
- \(PHALFL_{\text{FINAL}}\) = Final photolysis half-life in lakes
- \(PHALFL_{\text{D}}\) = Direct photolysis half-life in lakes
- \(PHALFL_{\text{I}}\) = Indirect photolysis half-life in lakes

\[
PHALFR_{\text{FINAL}} = \frac{1}{1 \div \text{PHALFR}_{\text{D}} + 1 \div \text{PHALFR}_{\text{I}}}
\]  
\(6\)

Where:
- \(PHALFR_{\text{FINAL}}\) = Final photolysis half-life in rivers
- \(PHALFR_{\text{D}}\) = Direct photolysis half-life in rivers
- \(PHALFR_{\text{I}}\) = Indirect photolysis half-life in rivers
3.3 Volatilization Half-Life

SCDM estimates the volatilization half-life in surface water for organic substances using Equation 7 (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 (T₁/₂) can be expressed as follows:

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

(7)

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:

\[ K_L (cm/hr) = \frac{(H / RT)k_g \times k_l}{(H / RT)k_g + k_l} \]  

(8)

Where:
H = Henry’s Law Constant (atm·m³/mol)
R = Universal gas constant (8.20 × 10⁻⁵ atm·m³/mol·K)
T = Temperature (K; ºC + 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:

\[ k_g (cm/hr) = 3,000 \times (18 / MW)^{1/2} \]  

(9)

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

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

(10)

Where:
V_{wind} = Wind velocity (m/s)
V_{curr} = Current velocity (m/s)

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

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

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

(11)

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

\[ k_1(m/s) = 23.51 \times (V_{\text{curr}}^{0.969} / (Z \times 1m / 100cm)^{0.673}) \times (32 / MW)^{1/2} \]  

(12)

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

\[ k_1(m/s) = 23.51 \times (V_{\text{curr}}^{0.969} / (Z \times 1m/100cm)^{0.673}) \times (32/MW)^{1/2}e^{0.526(V_{\text{wind}}^{-1.9})} \]  

(13)

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

Combining Equations (7), (8), (9), and (10) into a single equation for estimating volatilization half-life (\( T_{1/2} \)) for compounds with MW <65 g/mol gives the following equation:

\[ T_{1/2} (\text{days}) = \frac{18}{RT} \left( \frac{1}{(MW/44)^{1/2}} + \frac{RT}{(H \times 3000) \times (MW/18)^{1/2}} \right) \]  

(14)

The following equation, combining Equations (7), (8), (9), and (11), can be used to estimate the volatilization half-life (\( T_{1/2} \)) for compounds with MW \( \geq 65 \text{ g/mol} \) if the wind velocity is \( \leq 1.9 \text{ m/sec} \):

\[ T_{1/2} (\text{days}) = \frac{18}{RT} \left( \frac{1}{((Z \times \ln 2) \times [(Z \times 1m/100cm)^{0.673} / (23.51 \times V_{\text{curr}}^{0.969}) \times (MW / 32)^{1/2}] + RT \times (H \times 137.5 \times (V_{\text{wind}} + V_{\text{curr}})) \times (MW / 18)^{1/2}} \right) \]  

(15)

The following equation, combining Equations (7), (8), (9), and (12), can be used to estimate the volatilization half-life (\( T_{1/2} \)) for compounds with MW \( \geq 65 \text{ g/mol} \) if the wind velocity is \( > 1.9 \text{ m/sec} \) and \( \leq 5 \text{ m/sec} \):

\[ T_{1/2} (\text{days}) = \frac{18}{RT} \left( \frac{1}{((Z \times \ln 2) \times [(Z \times 1m/100cm)^{0.673} / (23.51 \times V_{\text{curr}}^{0.969}) \times (MW / 32)^{1/2}] e^{0.526(1.9-V_{\text{wind}})/5.137.5} + RT \times (H \times 137.5 \times (V_{\text{wind}} + V_{\text{curr}})) \times (MW / 18)^{1/2}} \right) \]  

(16)

If \( H < 10^{-7} \text{ atm} \cdot \text{m}^3 / \text{mol} \), the substance is less volatile than water and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, pp. 15-9 to 15-28) and no volatilization half-life is estimated for rivers or lakes.

### 3.3.1 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 (14) and (15) reduce to the following:

- If MW <65 g/mol:

\[ T_{1/2} (\text{days}) = 2.89 \times \{ [0.05 \times (MW / 44)^{1/2}] + [8.1 \times 10^{-6} / H] \times (MW / 18)^{1/2} \} \]  

(17)
3.3.2 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 (14) and (15) reduce to the following:

- If \( MW < 65 \text{ g/mol} \):
  \[
  T_{1/2} \text{ (days)} = 2.89 \times \left\{ \left[0.0425 \times (MW/32)^{1/2}\right] + \left[(1.4 \times 10^{-5} / H) \times (MW/18)^{1/2}\right] \right\}
  \]

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

- If \( MW \geq 65 \text{ g/mol} \):
  \[
  T_{1/2} \text{ (days)} = 2.89 \times \left\{ \left[0.0425 \times (MW/32)^{1/2}\right] + \left[(1.4 \times 10^{-5} / H) \times (MW/18)^{1/2}\right] \right\}
  \]

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

3.4 Overall Half-Lives

3.4.1 Surface Water Persistence Overall Half-Lives for Non-radiouclides

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

\[
\text{HALF}_LAK = \frac{1}{\text{HHALFL} + \text{BHALFL} + \text{PHALFL} + \text{VHALFL}}
\]

Where:
\( \text{HHALFL} = \text{Hydrolysis half-life in lakes} \)
\( \text{BHALFL} = \text{Biodegradation half-life in lakes} \)
\( \text{PHALFL} = \text{Photolysis half-life in lakes} \)
\( \text{VHALFL} = \text{Volatilization half-life in lakes} \)

\[
\text{HALF}_RIV = \frac{1}{\text{HHALFR} + \text{BHALFR} + \text{PHALFR} + \text{VHALFR}}
\]

Where:
\( \text{HHALFR} = \text{Hydrolysis half-life in rivers} \)
\( \text{BHALFR} = \text{Biodegradation half-life in rivers} \)
PHALFR = Photolysis half-life in rivers
VHALFR = Volatilization half-life in rivers

3.4.2 Surface Water Persistence 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):

\[
\text{HALF}_R\_LAK = \frac{1}{\frac{1}{\text{RHALFL}} + \frac{1}{\text{VHALFL}}}
\]

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

\[
\text{HALF}_R\_RIV = \frac{1}{\frac{1}{\text{RHALFR}} + \frac{1}{\text{VHALFR}}}
\]

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

3.4.3 SsI Degradation Overall Half-Lives for Non-radionuclides

SsI degradation overall half-lives are estimated for non-radioactive substances, as follows:

\[
\text{SSIHALF} = \frac{1}{\frac{1}{\text{SSIHHALF}} + \frac{1}{\text{SSIBHALF}}}
\]

Where:
SSIHHALF = SsI hydrolysis half-life
SSIBHALF = SsI biodegradation half-life

3.5 Soil Water Distribution Coefficient (Kd); Soil Organic/Carbon Partition Coefficients (Koc)

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 Kd value and its water solubility value. Kd 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:

\[
K_d = (K_{oc})(f_s)
\]

(26)

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:

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

(27)

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):

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

(28)

The determination of which equation is applied to each substance is also described in Section 2.8 of this methodology document. A \(K_{oc}\) Equation field value of 1 indicates that Equation 27 is applied, and a value of 2 indicates Equation 28 is applied.

### 3.6 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:

\[
\text{Geometric Mean Solubility} = \sqrt{(\text{low water solubility}) \times (\text{high water solubility})}
\]

(29)
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 and SsI Component

The following equations are used to determine air inhalation screening concentration benchmarks for the air migration pathway and SsI component. 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), Risk Assessment Guidance for Superfund, Part F (2009) and Exposure Factors Handbook (2011). 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 Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens. Equations used for radionuclides are provided in Section 4.1.5.

4.1.1 Non-carcinogenic – Air and SsI, Inhalation

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

(30)

Where:

- \(SC_{nc-air}\) = Air Inhalation Screening Concentration, Non-Carcinogenic (\(\mu g/m^3\))
- \(THQ\) = Target hazard quotient (\(=1\)), unitless
- \(AT\) = Averaging time (365 days/year)
- \(ED\) = Exposure duration (26 years)
- \(EF\) = Exposure frequency (350 days/year)
- \(ET\) = Exposure time (24 hours/day)
- \(RfC\) = Reference concentration (\(mg/m^3\))

Using the exposure assumptions listed above, Equation (30) can be simplified as:

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

(31)

4.1.2 Carcinogenic – Air and SsI, Inhalation

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

(32)
Where:

\[ SC_{\text{c-air}} = \text{Air Inhalation Screening Concentration, Carcinogenic (µg/m}^3\text{)} \]
\[ TR = \text{Target risk (1 x 10}^{-6}\text{)} \text{ (unitless)} \]
\[ AT = \text{Averaging time (365 days/}\text{year)} \]
\[ LT = \text{Lifetime (70 years)} \]
\[ ED = \text{Exposure duration (26 years)} \]
\[ EF = \text{Exposure frequency (350 days/}\text{year)} \]
\[ ET = \text{Exposure time (24 hours/}\text{day)} \]
\[ IUR = \text{Inhalation unit risk (µg/m}^3\text{)}^{-1} \]

Using the exposure assumptions listed above, Equation (32) can be simplified as:

\[ SC_{\text{c-air}} = \frac{2.808 \times 10^{-6}}{IUR} \quad (33) \]

### 4.1.3 Carcinogenic – Air and SsI, Inhalation – Asbestos

\[ SC_{\text{c-air-asbestos}} \text{ (fibers/mL)} = \frac{TR}{(IUR \times TWF)} \quad (34) \]

Where:

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

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

\[ SC_{\text{mu-air}} = \frac{TR \times (AT \times LT)}{EF \times ET \times \left( \frac{1 \text{ day}}{24 \text{ hours}} \right) \times [(ED_{0-2} \times IUR \times 10) + (ED_{2-6} \times IUR \times 3) + (ED_{6-16} \times IUR \times 3) + (ED_{16-26} \times IUR \times 1)]} \quad (35) \]

Where:

\[ SC_{\text{mu-air}} = \text{Air Inhalation Screening Concentration, Carcinogenic – Mutagenic Mode of Action (µg/m}^3\text{)} \]
\[ TR = \text{Target risk (1 x 10}^{-6}\text{)} \text{ (unitless)} \]
\[ AT = \text{Averaging time (365 days/}\text{year)} \]
\[ LT = \text{Lifetime (70 years)} \]
\[ ED_{0-2} = \text{Exposure duration – resident (2 years)} \]
\[ ED_{2-6} = \text{Exposure duration – resident (4 years)} \]
\[ ED_{6-16} = \text{Exposure duration – resident (10 years)} \]
\[ ED_{16-26} = \text{Exposure duration – resident (10 years)} \]
\[ EF = \text{Exposure frequency – resident (350 days/}\text{year)} \]
\[ ET = \text{Exposure time – resident (24 hours/}\text{day)} \]
\[ IUR = \text{Inhalation unit risk (µg/m}^3\text{)}^{-1} \]

Using the exposure assumptions listed above, Equation (35) can be simplified as:
\[
SC_{\text{mu-air}} = \frac{1.014 \times 10^{-6}}{IUR}
\]  

(36)

### 4.1.4.1 Vinyl Chloride – Air and SSI, Inhalation

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

(37)

**Where:**
- \(SC_{\text{mu-vc}}\) = 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 – resident (26 years)
- \(EF\) = Exposure frequency – resident (350 days/year)
- \(ET\) = Exposure time – resident (24 hours/day)
- \(IUR\) = Inhalation unit risk (µg/m³)⁻¹

Using the exposure assumptions listed above, Equation (37) can be simplified as:

\[
SC_{\text{mu-vc}} = \frac{7.374 \times 10^{-7}}{IUR}
\]  

(38)

### 4.1.4.2 Trichloroethylene – Air and SSI, 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.

\[
SC_{\text{mu-tce}} = \frac{TR \times (AT \times LT)}{EF \times ET \times (1 \text{ day/24 hours}) \times [(ED_{0-2} \times IUR_{\text{kidney}} \times 10) + (ED_{2-6} \times IUR_{\text{kidney}} \times 3) + (ED_{6-16} \times IUR_{\text{kidney}} \times 3) + (ED_{16-26} \times IUR_{\text{kidney}} \times 1)]}
\]  

(39)

**Where:**
- \(SC_{\text{mu-tce}}\) = 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 – resident (2 years)
- \(ED_{2-6}\) = Exposure duration – resident (4 years)
- \(ED_{6-16}\) = Exposure duration – resident (10 years)
- \(ED_{16-26}\) = Exposure duration – resident (10 years)
- \(EF\) = Exposure frequency – resident (350 days/year)
\( ET \) = Exposure time – resident (24 hours/day)
\( IUR_{\text{kidney}} \) = Inhalation unit risk, kidney (\( \mu g/m^3 \))\(^{-1} \)

Using the exposure assumptions listed above, Equation (39) can be simplified as:

\[
SC_{m-air} = 1.014 \times 10^{-6} / IUR_{\text{kidney}} \tag{40}
\]

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

\[
SC_{c-tce} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times (1 \text{ day/24 hours}) \times IUR_{\text{NHL and Liver}}} \tag{41}
\]

Where:

- \( SC_{c-tce} \) = Air Inhalation Screening Concentration, Carcinogenic (\( \mu g/m^3 \))
- \( TR \) = Target risk (1 \( \times 10^{-6} \)) (unitless)
- \( AT \) = Averaging time (365 days/year)
- \( LT \) = Lifetime (70 years)
- \( ED \) = Exposure duration – resident (26 years)
- \( EF \) = Exposure frequency – resident (350 days/year)
- \( ET \) = Exposure time – resident (24 hours/day)
- \( IUR_{\text{NHL and liver}} \) = Inhalation unit risk, NHL and liver (\( \mu g/m^3 \))\(^{-1} \)

Using the exposure assumptions listed above, Equation (41) can be simplified as:

\[
SC_{c-air} = 2.81 \times 10^{-6} / IUR_{\text{NHL and liver}} \tag{42}
\]

**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.

\[
SC_{mu-c-tce} = \frac{1}{SC_{m-air} + SC_{c-air}} \tag{43}
\]

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

\[
SC_{mu-c-tce} = \frac{1}{9.86 \times 10^5 IUR_{\text{kidney}} + 3.56 \times 10^5 IUR_{\text{NHL and Liver}}} \tag{44}
\]
4.1.5 Carcinogenic – Air, Inhalation and SsI, Radionuclides

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

(45)

Where:

\[ IFA_{r-adj} = \frac{(IRA_c \times ED_c + IRA_{a} \times ED_{a})}{ED} \]

\[ SC_{c-air-rad} = \text{Air inhalation screening concentration benchmark – radiochemical (pCi/m}^3) \]

\[ SF_i = \text{Slope factor – inhalation, radiochemical – substance specific (pCi)}^3 \]

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

\[ ET = \text{Exposure time – resident (24 hours/day)} \]

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

\[ ED = \text{Exposure duration – resident (26 years)} \]

\[ IRA_c = \text{Inhalation rate – resident child (10 m}^3/\text{day)} \]

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

\[ ED_{a} = \text{Exposure duration – resident adult (20 years)} \]

\[ IRA_{a} = \text{Inhalation rate – resident adult (20 m}^3/\text{day)} \]

\[ IFA_{r-adj} = \text{Age-adjusted inhalation factor (18 m}^3/\text{day)} \]

Using the exposure assumptions listed above, Equation (45) can be simplified as:

\[ SC_{c-air-rad} = 6.21 \times 10^{-12} / SF_i \]  

(46)

4.2 Screening Concentration Benchmarks for the Soil Exposure Component

The following equations are used to determine soil ingestion screening concentration benchmarks for the soil exposure component. 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) and Exposure Factors Handbook (2011). 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 Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens. 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

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

(47)

Where:

\[ SC_{res-sol-nc-ing} = \text{Soil Screening Concentration, Non-Carcinogenic (mg/kg)} \]
\[ RfD = \text{Reference dose (in mg/kg-day)} \]
\[ AT = \text{Averaging time – resident (365 days/year)} \]
\[ BM_c = \text{Body mass – child (= 15 kg)} \]
\[ ED_c = \text{Exposure duration – resident child (= 6 years)} \]
\[ EF = \text{Exposure frequency – resident (= 350 days/year)} \]
\[ IRS_c = \text{Resident soil ingestion rate – child (= 200 mg/day)} \]
\[ THQ = \text{Target hazard quotient (=1)} \]

Using the exposure assumptions listed above, Equation (47) can be simplified as:

\[ SC_{\text{res-sol-ing}} = 78214.29 \times RfD \quad (48) \]

### 4.2.2 Carcinogenic – Soil, Ingestion

\[ SC_{\text{res-sol-ca-ing}} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times 10^{-6} \text{ kg}} \quad (49) \]

Where:

\[ SC_{\text{res-sol-ca-ing}} = \text{Soil Screening Concentration, Carcinogenic (mg/kg)} \]
\[ IFS = \text{Soil ingestion rate – resident, age adjusted [= (105 mg-year) / (kg-day)], calculated as:} \]

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

\[ SF = \text{Slope factor (mg/kg-day)}^{-1} \]
\[ TR = \text{Target risk (= 1 x 10^{-6})} \]
\[ AT = \text{Averaging time – resident (365 days/year)} \]
\[ LT = \text{Lifetime (= 70 years)} \]
\[ EF = \text{Exposure frequency – resident (= 350 days/year)} \]
\[ ED_r = \text{Exposure duration – resident (= 26 years)} \]
\[ IRS_a = \text{Resident soil ingestion rate – adult (= 100 mg/day)} \]
\[ IRS_c = \text{Resident soil ingestion rate – child (= 200 mg/day)} \]
\[ BM_a = \text{Body mass – adult (= 80 kg)} \]
\[ BM_c = \text{Body mass – child (= 15 kg)} \]

Using the exposure assumptions listed above, Equation (49) can be simplified as:

\[ SC_{\text{res-sol-ca-ing}} = \frac{0.695}{SF} \quad (50) \]

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

\[ SC_{\text{res-sol-mu-ing}} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times 10^{-6} \text{ kg}} \quad (51) \]
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 [= (476.7 mg-year) / (kg-day)], calculated as:

$$IFSM = \left( \frac{ED_{0-2} \times IRS_c \times 10}{BM_c} \right) + \left( \frac{ED_{2-6} \times IRS_c \times 3}{BM_c} \right) + \left( \frac{ED_{6-16} \times IRS_a \times 3}{BM_a} \right) + \left( \frac{ED_{16-26} \times IRS_a \times 1}{BM_a} \right)$$

$SF$ = Slope factor (mg/kg-day)$^{-1}$

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

$AT$ = Averaging time – resident (= 365 days/year)

$LT$ = Lifetime (= 70 years)

$EF$ = Exposure frequency – resident (= 350 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)

$ED_{16-26}$ = Exposure duration – resident ages 16-26 (= 10 years)

$IRS_a$ = Resident soil ingestion rate – adult (= 100 mg/day)

$IRS_c$ = Resident soil ingestion rate – child (= 200 mg/day)

$BM_a$ = Body mass – adult (= 80 kg)

$BM_c$ = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (51) can be simplified as:

$$SC_{\text{res-sol-mu-ing}} = \frac{0.153}{SF}$$

(52)

4.2.3.1 Vinyl Chloride – Soil, Ingestion

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

(53)

Where:

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

$IFS$ = Soil ingestion rate – resident, age adjusted [= (105 mg-year) / (kg-day)], calculated as:

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

$SF$ = Slope factor (mg/kg-day)$^{-1}$

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

$AT$ = Averaging time – resident (= 365 days/year)

$LT$ = Lifetime (= 70 years)

$EF$ = Exposure frequency – resident (= 350 days/year)

$ED_c$ = Exposure duration – child (= 6 years)

$ED_r$ = Exposure duration – resident (= 26 years)

$IRS_a$ = Resident soil ingestion rate – adult (= 100 mg/day)
Using the exposure assumptions listed above, Equation (53) can be simplified as:

$$SC_{res-sol-ca-vc-ing} = \frac{0.068}{SF}$$ (54)

### 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.

$$SC_{sol-mu-tce-ing} = \frac{TR \times AT \times LT}{SF_{kidney} \times EF \times IFSM \times \frac{10^{-6} \text{kg}}{\text{mg}}}$$ (55)

Where:

- $SC_{sol-mu-tce-ing} =$ Soil Screening Concentration, Mutagenic (mg/kg)
- $IFSM =$ Mutagenic soil ingestion rate–resident, age adjusted [= (476.7 mg-year)/(kg-day)], calculated as:

  $$IFSM = \left( \frac{ED_{0-2} \times IRS_c \times 10}{BM_c} \right) + \left( \frac{ED_{2-6} \times IRS_a \times 3}{BM_c} \right) + \left( \frac{ED_{6-16} \times IRS_a \times 3}{BM_a} \right) + \left( \frac{ED_{16-26} \times IRS_a \times 1}{BM_a} \right)$$

- $SF_{kidney} =$ Slope factor, kidney (mg/kg-day)$^{-1}$
- $TR =$ Target risk (= $1 \times 10^{-6}$)
- $AT =$ Averaging time – resident (= 365 days/year)
- $LT =$ Lifetime (= 70 years)
- $EF =$ Exposure frequency – resident (= 350 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)
- $ED_{16-26} =$ Exposure duration – resident ages 16-26 (= 10 years)
- $IRS_a =$ Resident soil ingestion rate – adult (= 100 mg/day)
- $IRS_c =$ Resident soil ingestion rate – child (= 200 mg/day)
- $BM_a =$ Body mass – adult (= 80 kg)
- $BM_c =$ Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (55) can be simplified as:

$$SC_{sol-mu-tce-ing} = \frac{0.153}{SF_{kidney}}$$ (56)

**Step 2.** A cancer screening concentration (SC) is calculated using the NHL and liver cancer slope factor and the cancer equation provided below.
Where:

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

(57)

\[ SC_{\text{sol-ca-tce-ing}} = \text{Soil Screening Concentration, Carcinogenic (mg/kg)} \]

\[ IFS = \text{Soil ingestion rate – resident, age adjusted [= (105 mg-year) / (kg-day)]}, \text{calculated as:} \]

\[ = \left( \frac{EDc \times IRS_c}{BM_c} \right) + \left[ \frac{(EDr - EDc) \times IRS_a}{BM_a} \right] \]

\[ SF_{\text{NHL and liver}} = \text{Slope factor, NHL and liver (mg/kg-day)}^{-1} \]

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

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

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

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

\[ ED_r = \text{Exposure duration – resident (= 26 years)} \]

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

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

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

\[ BM_a = \text{Body mass – adult (= 80 kg)} \]

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

Using the exposure assumptions listed above, Equation (57) can be simplified as:

\[ SC_{\text{sol-ca-tce-ing}} = \frac{0.695}{SF_{\text{NHL and Liver}}} \]  

(58)

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.

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

(59)

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:

\[ SC_{\text{soil-ca-mu-tce-ing}} = \frac{1}{1.44 SF_{\text{NHL and liver}} + 6.54 SF_{\text{kidney}}} \]  

(60)
4.2.4 Carcinogenic – Soil, Radionuclides

4.2.4.1 Oral

\[
SC_{c-sol-rad} = \frac{TR \times t_r \times \lambda}{(1-e^{-2\lambda t_r}) \times SF_s \times IFS_{r-adj} \times EF_r \times ED_r \times \left(\frac{g}{1000mg}\right)}
\]  

(61)

Where:

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

\[SC_{c-sol-rad} = \text{Soil cancer screening concentration benchmark – radiochemical (pCi/kg)}\]
\[SF_s = \text{Slope factor – soil, radiochemical – substance specific (pCi)}^{-1}\]
\[IFS_{r-adj} = \text{Resident soil ingestion factor (mg/day)}\]
\[TR = \text{Target risk (1 x 10^{-6})}\]
\[t_r = \text{Time (26 years)}\]
\[\lambda = \text{Lambda – substance specific}\]
\[EF_r = \text{Exposure frequency – resident (350 days/year)}\]
\[ED_r = \text{Exposure duration – resident (26 years)}\]
\[IRS_a = \text{Soil ingestion rate – adult (100 mg/day)}\]
\[IRS_c = \text{Soil ingestion rate – child (200 mg/day)}\]
\[ED_{c} = \text{Exposure duration – resident child (6 years)}\]
\[ED_{r-a} = \text{Exposure duration – resident adult (20 years)}\]

Using the exposure assumptions listed above, Equation (61) can be simplified as:

\[
SC_{c-sol-rad} = 2.32 \times 10^{-8} \times \lambda \times [(1 - e^{-26\lambda}) \times SF_s]
\]  

(62)

4.2.4.2 External Exposure (gamma emitters)

\[
SC_{ext-rad} = \frac{TR \times t_r \times \lambda}{(1-e^{-2\lambda t_r}) \times SF_{ext} \times ACF \times EF \times \left(\frac{1 \text{ year}}{365 \text{ days}}\right) \times ED \times [ET_{r-o} \times GSF_o + (ET_{r-i} \times GSF_{i})]}
\]  

(63)

Where:

\[SC_{ext-rad} = \text{Screening concentration benchmark – radiochemical, external (pCi/g)}\]
\[SF_{ext} = \text{Slope factor – external exposure – substance specific) (risk/yr per pCi/g)}\]
\[TR = \text{Target risk (= 1 x 10^{-6})}\]
\[t_r = \text{Time (26 years)}\]
\[\lambda = \text{Lambda – substance specific}\]
\[e = \text{Euler’s number (= 2.718281828)}\]
\[ACF = \text{Area correction factor – substance specific}\]
\[EF = \text{Exposure frequency – resident (350 days/year)}\]
\[ED = \text{Exposure duration – resident (26 years)}\]
\[ED_{c} = \text{Exposure duration – resident child (6 years)}\]
\[ED_{r-a} = \text{Exposure duration – resident adult (20 years)}\]
\[ET_{r-o} = \text{Exposure time – resident outdoor (0.073 hr/hr)}\]
Using the exposure assumptions listed above, Equation (63) can be simplified as:

$$SC_{ext-rad} = \frac{2.60 \times 10^{-6} \times \lambda}{[(1 - e^{-2\lambda}) \times SF_{ext} \times ACF]}$$

(64)

4.3 Screening Concentration Benchmarks for Ground Water and Drinking Water

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 Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens. Equations used for radionuclides are provided in Section 4.3.4.

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

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

(65)

Where:
- $SC_{water-nc-ing} =$ Ground Water/Drinking Water Screening Concentration, Non-Carcinogenic (µg/L)
- $RfD =$ 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 (= 0.78 L/day)
- $THQ =$ Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (65) can be simplified as:

$$SC_{water-nc-ing} = 20054.95 \times RfD$$

(66)

4.3.2 Carcinogenic – Ground Water and Drinking Water, Ingestion

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

(67)
Where:

\( SC_{\text{water-ca-ing}} \) = Ground Water/Drinking Water Screening Concentration, Carcinogenic (µg/L)

\( IFW \) = Drinking water ingestion rate – Resident, adjusted \([= (0.937 \text{ L-year}) / (\text{kg-day})]\), calculated as:

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

\( SF \) = 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 \( (= 26 \text{ years}) \)

\( IRW_a \) = Drinking water ingestion rate – resident adult \( (= 2.5 \text{ L/day}) \)

\( IRW_c \) = Drinking water ingestion rate – resident child \( (= 0.78 \text{ L/day}) \)

\( BM_a \) = Body mass – adult \( (= 80 \text{ kg}) \)

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

Using the exposure assumptions listed above, Equation (67) can be simplified as:

\[
SC_{\text{water-ca-ing}} = \frac{0.0779}{SF}
\] (68)

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

\[
SC_{\text{water-mu-ing}} = \frac{TR \times AT \times LT \times 1000 \ \mu g/mg}{SF \times EF \times IFWM}
\] (69)

Where:

\( SC_{\text{water-mu-ing}} \) = Ground Water/Drinking Water Screening Concentration, Mutagenic (µg/L)

\( IFWM \) = Mutagenic Drinking Water ingestion rate – resident, age adjusted \([= (2.914 \text{ L-year}) / (\text{kg-day})]\), calculated as:

\[
IFWM = \left( \frac{ED_{0-2} \times IRW_{c} \times 10}{BM_c} \right) + \left( \frac{ED_{2-6} \times IRW_{c} \times 3}{BM_c} \right) + \left( \frac{ED_{6-16} \times IRW_{a} \times 3}{BM_a} \right) + \left( \frac{ED_{16-26} \times IRW_{a} \times 1}{BM_a} \right)
\]

\( SF \) = 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 \( (= 10 \text{ years}) \)

\( ED_{16-26} \) = Exposure duration – resident ages 16-26 \( (= 10 \text{ years}) \)

\( IRW_a \) = Drinking water ingestion rate – resident adult \( (= 2.5 \text{ L/day}) \)

\( IRW_c \) = Drinking water ingestion rate – resident child \( (= 0.78 \text{ L/day}) \)

\( BM_a \) = Body mass – adult \( (= 80 \text{ kg}) \)
Using the exposure assumptions listed above, Equation (69) can be simplified as:

\[
SC_{\text{water-mu-ing}} = \frac{0.0251}{SF}\tag{70}
\]

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

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

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 \([= (0.937 \text{ L-year}) / (\text{kg-day})]\), calculated as:
  \[
  \left(\frac{ED_c \times IRW_c}{BM_c}\right) + \left(\frac{(ED_r - ED_c) \times IRW_a}{BM_a}\right)
  \]
- \(SF\) = 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 \((= 26 \text{ years})\)
- \(IRW_a\) = Drinking water ingestion rate – resident adult \((= 2.5 \text{ L/day})\)
- \(IRW_c\) = Drinking water ingestion rate – resident child \((= 0.78 \text{ L/day})\)
- \(BM_a\) = Body mass – adult \((= 80 \text{ kg})\)
- \(BM_c\) = Body mass – child \((= 15 \text{ kg})\)

Using the exposure assumptions listed above, Equation (71) can be simplified as:

\[
SC_{\text{res-water-ca-vc-ing}} = \frac{0.0154}{SF}\tag{72}
\]

### 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.
\[
SC_{\text{water-mu-tce-ing}} = \frac{TR \times AT \times LT \times 1000 \mu g/mg}{SF_{\text{kidney}} \times EF \times IFWM}
\tag{73}
\]

Where:
- \(SC_{\text{water-mu-tce-ing}}\) = Drinking Water Screening Concentration, Mutagenic Mode of Action (\(\mu g/L\))
- \(IFWM\) = Mutagenic Drinking Water ingestion rate – resident, age adjusted \([= (2.914 \text{ L-year}) / (\text{kg-day})]\), calculated as:
  \[
  IFWM = (BM_{a} \times IRW_{a}) \times \left[\left(ED_{0-2} \times IRW_{c} \times 10 \div BM_{c}\right) + \left(ED_{2-6} \times IRW_{c} \times 3 \div BM_{c}\right) + \left(ED_{6-16} \times IRW_{c} \times 3 \div BM_{a}\right) + \left(ED_{16-26} \times IRW_{a} \times 1 \div BM_{a}\right)\right]
  \]
- \(SF_{\text{kidney}}\) = 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 \((= 10 \text{ years})\)
- \(ED_{16-26}\) = Exposure duration – resident ages 16-26 \((= 10 \text{ years})\)
- \(IRW_{c}\) = Drinking water ingestion rate – resident child \((= 0.78 \text{ L/day})\)
- \(IRW_{a}\) = Drinking water ingestion rate – resident adult \((= 2.5 \text{ L/day})\)
- \(BM_{c}\) = Body mass – child \((= 15 \text{ kg})\)
- \(BM_{a}\) = Body mass – adult \((= 80 \text{ kg})\)

Using the exposure assumptions listed above, Equation (73) can be simplified as:

\[
SC_{\text{water-mu-tce-ing}} = 0.0251 / SF_{\text{kidney}}
\tag{74}
\]

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

\[
SC_{\text{water-ca-tce-ing}} = \frac{TR \times AT \times LT \times 1000 \mu g/mg}{SF_{\text{NHL and Liver}} \times EF \times IFW}
\tag{75}
\]

Where:
- \(SC_{\text{water-ca-tce-ing}}\) = Drinking Water Screening Concentration, Carcinogenic (\(\mu g/L\))
- \(IFW\) = Drinking water ingestion rate – Resident, adjusted \([= (0.937 \text{ L-year}) / (\text{kg-day})]\), calculated as:
  \[
  IFW = (BM_{a} \times IRW_{a}) \times \left[\left(ED_{c} \times IRW_{c} \div BM_{c}\right) + \left[(ED_{c} - ED_{r}) \times IRW_{a} \div BM_{a}\right]\right]
  \]
- \(SF_{\text{NHL and liver}}\) = 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 \((= 350 \text{ days/year})\)
- \(ED_{c}\) = Exposure duration – child \((= 6 \text{ years})\)
- \(ED_{r}\) = Exposure duration – resident \((= 26 \text{ years})\)
- \(IRW_{a}\) = Drinking water ingestion rate – resident adult \((= 2.5 \text{ L/day})\)
Using the exposure assumptions listed above, Equation (75) can be simplified as:

$$SC_{\text{water-ca-tce-ing}} = 0.0779 / SF_{\text{NHL and liver}}$$  \hspace{1cm} (76)

**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.

$$SC_{\text{water-ca-mu-ice-ing}} = \frac{1}{\left(\frac{1}{SC_{\text{water-ca-ing}}}\right) + \left(\frac{1}{SC_{\text{water-mu-ing}}}\right)}$$  \hspace{1cm} (77)

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative to Equation 76 for calculating Step 3 results:

$$SC_{\text{water-ca-mu-ice-ing}} = \frac{1}{12.82 SF_{\text{NHL and Liver}} + 39.84 SF_{\text{kidney}}}$$  \hspace{1cm} (78)

### 4.3.4 Carcinogenic – Ground Water and Drinking Water, Radionuclides

$$SC_{c-water-rad} = \frac{TR}{EF_r \times ED_r \times SF_w \times IFW_{r-adj}}$$  \hspace{1cm} (79)

**Where:**

$$IFW_{r-adj} = \frac{ED_c \times IRW_c + ED_{r-a} \times IRW_a}{ED_r}$$

- $SC_{c-water-rad}$ = Drinking water screening concentration benchmark – radiochemical (pCi/L)
- $SF_w$ = Slope factor – drinking water – substance specific (pCi)$^{-1}$
- $TR$ = Target risk (1 x 10$^{-6}$), unitless
- $EF_r$ = Exposure frequency – resident (350 days/year)
- $ED_r$ = Exposure duration – resident (26 years)
- $IRW_a$ = Water ingestion rate – adult (2.5 L/day)
- $IRW_c$ = Water ingestion rate – child (0.78 L/day)
- $ED_{r-a}$ = Exposure duration – resident adult (20 years)
- $IFW_{r-adj}$ = Age-adjusted water ingestion rate (2.1 L/day)

Using the exposure assumptions listed above, Equation (79) can be simplified as:
SC_{water-rad} = 5.23 \times 10^{-11} / SF_w \tag{80}

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

The following equations are used to determine screening concentration benchmarks for the human food chain threat. 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

\[
SC_{res-fish-nc-ing} = \frac{THQ \times AT \times ED_r \times BM_a}{EF \times ED_r \times \left(1 + 10^{-6}\right) \times IRF \times \frac{10^{-6} \text{ kg}}{\text{mg}}} \tag{81}
\]

Where:
- \(SC_{res-fish-nc-ing}\) = Human Food Chain Screening Concentration, Fish Ingestion, Non-Carcinogenic (mg/kg)
- \(RfD\) = Reference dose (in mg/kg-day)
- \(AT\) = Averaging time – resident (365 days/year)
- \(BM_a\) = Body mass – adult (= 80 kg)
- \(ED_r\) = Exposure duration – resident (= 26 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 (81) can be simplified as:

\[
SC_{res-fish-nc-ing} = 1540 \times RfD \tag{82}
\]

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

\[
SC_{res-fish-ca-ing} = \frac{TR \times AT \times LT \times BM_a}{EF \times ED_r \times SF \times IRF \times \frac{10^{-6} \text{ kg}}{\text{mg}}} \tag{83}
\]

Where:
- \(SC_{res-fish-ca-ing}\) = Human Food Chain Screening Concentration, Fish Ingestion, Carcinogenic (mg/kg)
- \(SF\) = Slope factor (mg/kg-day)^{-1}
- \(TR\) = Target risk (= 1 x 10^{-6})
- \(AT\) = Averaging time – resident (= 365 days/year)
- \(LT\) = Lifetime (= 70 years)
- \(BM_a\) = Body mass – adult (= 80 kg)
- \(EF\) = Exposure frequency – resident (= 350 days/year)
- \(ED_r\) = Exposure duration – resident (= 26 years)
- \(IRF\) = Fish ingestion rate (= 5.4 x 10^4 mg / day)
Using the exposure assumptions listed above, Equation (83) can be simplified as:

\[
SC_{res\_fsh\_ca\_ing} = \frac{0.00416}{SF}
\]  

(84)

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

\[
SC_{c\_fsh\_rad} = \frac{TR}{EF_r \times ED \times SF_f \times IRF \times \frac{g}{1000 \text{mg}}}
\]  

(85)

Where:

- \(SC_{c\_fsh\_rad}\) = 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
- \(EF_r\) = Exposure frequency – resident (350 days/year)
- \(ED\) = Exposure duration – resident (26 years)
- \(ED_c\) = Exposure duration – resident child (6 years)
- \(ED_{ra}\) = Exposure duration – resident adult (20 years)
- \(IRF\) = Fish ingestion rate (= 5.4 \times 10^4 \text{ mg / day})

Using the exposure assumptions listed above, Equation (85) can be simplified as:

\[
SC_{c\_fsh\_rad} = 2.04 \times 10^{-12} / SF_f
\]  

(86)
5.0 SCDM DATA REPORTING and WEB QUERY

5.1 Data Reporting

Data are collected from the references identified in Section 2 of this document. With the exceptions cited in Section 2.1, 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 the SCDM Web Query.

The following rules are applied for purposes of reporting SCDM data in the SCDM Web Query:

- Substance characterization data and data that serve as inputs to benchmark and factor value formulas are rounded and reported to three figures.
- Screening concentration benchmarks are rounded and reported to three figures. Although this sometimes results in more figures than contained in the input variable (e.g., RfD, RfC, SF, or IUR) used to determine each benchmark, the additional figures are provided to assist users in checking the math.
- 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, 55 FR 51532, and 82 FR 2760.

5.2 SCDM Web Query

The SCDM Web Query (http://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm-query) contains selected data, HRS factor values and benchmarks for each hazardous substance in SCDM. Information is provided in tables for each substance. These tables are divided into three categories of available information: factor values, benchmarks and data elements.

Figure 1 presents an example of the header that appears on the SCDM Web Query report for each substance. The header contains the substance name, the substance CASRN, and the date the query is accessed.

![Figure 1. SCDM Web Query Report Heading](http://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm-query)

For each substance, the data elements tables contain all of the selected chemical data, the data units, and an abbreviation describing the reference source of the information. The reference source abbreviations are provided alongside corresponding reference list citations in Section 6 of this methodology document. A reference source value of “CALC” indicates that a value was calculated using other collected data, and a reference source value of “HRS” indicates a value prescribed by the HRS. Data are divided into seven functional groups: toxicity, persistence, SSI degradation, mobility, bioaccumulation, physical characteristics, other data and class information.

The toxicity table (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 human toxicity and ecotoxicity factor values.
### Data Elements: Toxicity

**Acenaphthene [CASRN 000083-32-9]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>RfD</td>
<td>6.00E-02</td>
<td>mg/kg/day</td>
<td>IRIS</td>
</tr>
<tr>
<td>RfC</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Slope Factor</td>
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</tr>
<tr>
<td>Slope Factor WOE</td>
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<td>--</td>
<td>--</td>
</tr>
<tr>
<td>IUR</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>IUR WOE</td>
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<td>--</td>
</tr>
<tr>
<td>Oral ED₁₀ WOE</td>
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<td>--</td>
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</tr>
<tr>
<td>Inhalation ED₁₀</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Inhalation ED₁₀ WOE</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
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<tr>
<td>Acute, Saltwater CMC</td>
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<td>--</td>
</tr>
<tr>
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<td>--</td>
</tr>
<tr>
<td>Chronic, Saltwater CCC</td>
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<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Freshwater Ecological LC₅₀</td>
<td>5.00E+01</td>
<td>μg/L</td>
<td>ECOTOX</td>
</tr>
<tr>
<td>Saltwater Ecological LC₅₀</td>
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<td>μg/L</td>
<td>ECOTOX</td>
</tr>
</tbody>
</table>

**Figure 2a. Non-radionuclide Toxicity Table**
Data Elements: Toxicity

Cadmium 109 (radionuclide) [CASRN 014109-32-1]

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<th>Source</th>
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</tr>
<tr>
<td>RfC</td>
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<tr>
<td>Oral Slope Factor, Food</td>
<td>6.70E-12</td>
<td>pCi(^{-1})</td>
<td>OSRTI_PRG</td>
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<tr>
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<td>pCi(^{-1})</td>
<td>OSRTI_PRG</td>
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<td>pCi(^{-1})</td>
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</tr>
<tr>
<td>Oral Slope Factor WOE</td>
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<td>--</td>
<td>HRS</td>
</tr>
<tr>
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<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>IUR WOE</td>
<td>A</td>
<td>--</td>
<td>HRS</td>
</tr>
<tr>
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<td>pCi(^{-1})</td>
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</tbody>
</table>

Figure 2b. Radionuclide Toxicity Table

The top half of the table shown in Figure 2a contains the data used for non-radionuclides to determine the HTF value: reference dose, reference concentration, slope factor, 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 the Figure 2a table 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 table shown in Figure 2b includes similar parameters for radionuclides.

The persistence table (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).

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<td>CALC</td>
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<td>--</td>
</tr>
<tr>
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<td>days</td>
<td>--</td>
</tr>
<tr>
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<td>HEDR</td>
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<tr>
<td>Radioactive</td>
<td>--</td>
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</tr>
</tbody>
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<table>
<thead>
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<th>Parameter</th>
<th>Value</th>
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<tbody>
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</table>

**Figure 3. Persistence Table**

The SsI degradation table (Figure 4) contains the SsI degradation data compiled using the methodology described in Section 2.4 of this methodology document. Along with additional site-specific data, these parameters are used to generate site-specific SsI degradation factor values that are not included in SCDM.
The mobility table (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. K_{OC} is used in determining K_{d}.

The bioaccumulation table (Figure 6) contains the human food chain and environmental bioaccumulation potential factor data compiled using the methodology described in Section 2.5 of this methodology document. 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.
### Data Elements: Bioaccumulation

**Acenaphthene [CASRN 000083-32-9]**

#### FOOD CHAIN

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<th>Parameter</th>
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#### ENVIRONMENTAL

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</tr>
<tr>
<td>Saltwater BCF</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

#### OTHER

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log K&lt;sub&gt;ow&lt;/sub&gt;</td>
<td>3.92E+00</td>
<td></td>
<td>EPI_EXP</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>3.90E+00</td>
<td>mg/L</td>
<td>PHYSPROP</td>
</tr>
<tr>
<td>Geometric Mean Solubility</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

**Figure 6. Bioaccumulation Table**

The physical characteristics table (Figure 7) contains logical “yes/no” flags that classify the substance based on physical properties and other aspects as described in Section 2.8 of this methodology document. MW is used to determine volatilization half-life.

### Data Elements: Physical Characteristics

**Acenaphthene [CASRN 000083-32-9]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal Containing</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Organic</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Air Pathway Gas</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Air Pathway Particulate</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>SSL Volatile</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Radionuclide</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Radioactive Element</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Mutagen</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>1.54E+02</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>1.22E+00</td>
<td>g/mL @ 20.0 °C</td>
</tr>
</tbody>
</table>

**Figure 7. Physical Characteristics Table**
The table labeled “other data” (Figure 8) contains values for melting points and boiling points (°C). The chemical formula is also listed here. Finally, the KOC equation parameter identifies which equation is used in generating a KOC from a KOW when no KOC is available from references.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point</td>
<td>9.34E+01</td>
<td>°C</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>2.79E+02</td>
<td>°C</td>
</tr>
<tr>
<td>Formula</td>
<td>C12H10</td>
<td></td>
</tr>
<tr>
<td>KOC Equation</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Figure 8. Other Data Table

The class information table (Figure 9) 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, Kd, and geometric mean water solubility. The “other” class includes hydrolysis, biodegradation, photolysis and volatilization half-lives, as well as BCFs and Log KOW. This section may also list other class-parent chemical substitutions for specific data elements.

The two main groups of substances involved in the majority of instances of inheriting data from a parent substance are 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.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parent Substance</td>
<td>--</td>
</tr>
</tbody>
</table>

Figure 9. Class Information Table

The other two categories of SCDM Web Query tables—factor values and benchmarks—contain the factor values (Figures 10 through 14) and benchmarks (Figures 15 through 17) required by the HRS. SCDM determines factor values using HRS methodologies from selected data in the data elements tables. The factor values are presented by HRS pathway: ground water, surface water, the two components of the soil exposure and subsurface intrusion pathway (soil exposure component and SsI component), and air. 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/components. 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 the SsI component, vapor migration potential is used to determine likelihood of exposure, SsI overall half-life and radioactive half-life are used in determining the site-specific degradation factor value, and SsI volatility is used to indicate a substance’s eligibility in several aspects of the SsI component evaluation. The air pathway gas migration factor value is used to determine
likelihood of release. For radioactive substances, human toxicity, ecosystem toxicity and surface water persistence factor values are determined as specified in Section 7 of the HRS.

**Factor Values: Ground Water Pathway**
*Acenaphthene [CASRN 000083-32-9]*

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicity</td>
<td>10</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>3.90E+00</td>
</tr>
<tr>
<td>Distribution Coefficient</td>
<td>7.64E+02</td>
</tr>
<tr>
<td>Geometric Mean Solubility</td>
<td>--</td>
</tr>
<tr>
<td>Mobility: Liquid, Karst</td>
<td>1.0E+00</td>
</tr>
<tr>
<td>Mobility: Liquid, Non-Karst</td>
<td>1.0E-02</td>
</tr>
<tr>
<td>Mobility: Non-Liquid, Karst</td>
<td>2.0E-01</td>
</tr>
<tr>
<td>Mobility: Non-Liquid, Non-Karst</td>
<td>2.0E-03</td>
</tr>
</tbody>
</table>

**Figure 10. Ground Water Pathway Factor Values Table**

**Factor Values: Surface Water Pathway**
*Acenaphthene [CASRN 000083-32-9]*

**DRINKING WATER**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicity</td>
<td>10</td>
</tr>
<tr>
<td>Persistence, River</td>
<td>0.4</td>
</tr>
<tr>
<td>Persistence, Lake</td>
<td>0.07</td>
</tr>
</tbody>
</table>

**HUMAN FOOD CHAIN**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicity</td>
<td>10</td>
</tr>
<tr>
<td>Persistence, River</td>
<td>0.4</td>
</tr>
<tr>
<td>Persistence, Lake</td>
<td>0.07</td>
</tr>
<tr>
<td>Bioaccumulation, Freshwater</td>
<td>500</td>
</tr>
<tr>
<td>Bioaccumulation, Saltwater</td>
<td>500</td>
</tr>
</tbody>
</table>

**ENVIRONMENTAL**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicity, Freshwater</td>
<td>10000</td>
</tr>
<tr>
<td>Toxicity, Saltwater</td>
<td>1000</td>
</tr>
<tr>
<td>Persistence, River</td>
<td>0.4</td>
</tr>
<tr>
<td>Persistence, Lake</td>
<td>0.07</td>
</tr>
<tr>
<td>Bioaccumulation, Freshwater</td>
<td>500</td>
</tr>
<tr>
<td>Bioaccumulation, Saltwater</td>
<td>500</td>
</tr>
</tbody>
</table>

**Figure 11. Surface Water Pathway Factor Values Table**
The benchmarks (Figures 15 through 20), like the factor values, are presented by pathway: ground water, surface water, the two components of the soil exposure and subsurface intrusion pathway (soil exposure component and SsI component), and air, as described in Sections 3 through 6 of the HRS. 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: Surface Water Pathway

**Acenaphthene [CASRN 000083-32-9]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCL</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>MCLG</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Non-Cancer Risk</td>
<td>1.20E+00</td>
<td>mg/L</td>
</tr>
</tbody>
</table>

**HUMAN FOOD CHAIN**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDAAL</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Non-Cancer Risk</td>
<td>9.27E+01</td>
<td>mg/kg</td>
</tr>
</tbody>
</table>

**ENVIRONMENTAL**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute, Freshwater CMC</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Acute, Saltwater CMC</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Chronic, Freshwater CCC</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Chronic, Saltwater CCC</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

Figure 16. Surface Water Pathway Benchmarks Table

### Benchmarks: Soil Exposure Component

**Acenaphthene [CASRN 000083-32-9]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Non-Cancer Risk</td>
<td>4.69E+03</td>
<td>mg/kg</td>
</tr>
</tbody>
</table>

Figure 17. Soil Exposure Component Benchmarks Table

### Benchmarks: Subsurface Intrusion Component

**Acenaphthene [CASRN 000083-32-9]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Non-Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

Figure 18. Subsurface Intrusion Component Benchmarks Table
### Benchmarks: Air Pathway

**Acenaphthene [CASRN 000083-32-9]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>NAAQS</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>NESHAPS</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Non-Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

*Figure 19. Air Pathway Benchmarks Table*

### Benchmarks: Radionuclide

**Acenaphthene [CASRN 000083-32-9]**

**DRINKING WATER**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCL</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

**HUMAN FOOD CHAIN**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

**SOIL**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>UMTRCA</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Cancer Risk Soil Ingestion</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Cancer Risk Soil Gamma</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

**SUBSURFACE INTRUSION**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

**AIR**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer Risk</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

*Figure 20. Radionuclide Benchmarks Table*
6.0 REFERENCES

References cited in the data collection hierarchies are listed below, along with references that have been consulted for general information. For references that may be cited in the “Source” field of the SCDM Web Query tables, the corresponding abbreviation is listed in square brackets.


- ATSDR minimal risk levels (MRLs). http://www.atsdr.cdc.gov/mrls/mrllist.asp [ATSDR for MRLs; ATSDR-Int for intermediate MRLs]


- California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp. [CALEPA]


• **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/tsca-screening-tools/epi-suite-estimation-program-interface. [EPI_EST for estimated values; EPI_EXP for experimental values]


• Syracuse Research Corporation (SRC), **PHYSPROP Database**. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html. [PHYSPROP]


July 2020


- U.S. EPA. *ECOTOX Database*. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/chemical-research/ecotoxicology-database. [ECOTOX]


  Primary PRG source documents include:
  
  

• U.S. EPA. *Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs)* derived by the EPA's Superfund Health Risk Technical Support Center (STSC) for the EPA Superfund program. http://hhpprtv.ornl.gov. [PPRTV; PPRTV-Sub for subchronic values]

• U.S. EPA. *Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs), Derivation Support Documents*. https://hhpprtv.ornl.gov/quickview/pprtv_papers.php. [PPRTV_APPENDIX; PPRTV_APP-Sub for subchronic values]

