

3.0 CALCULATIONS IN SCDM

3.1 Volatilization Half-Life

SCDM estimates volatilization half-life in surface water for organic substances using Equation 15-12 from Thomas (1990). In this method, the volatilization half-life ($\tau_{1/2}$) can be expressed as follows:

$$\tau_{1/2} = \frac{Z \times \ln 2}{K_L \text{ hr}} \quad (6)$$

where:

- Z = Mean water body depth (cm)
- K_L = Overall liquid-phase mass transfer coefficient.

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

$$K_L = \frac{(H/RT)k_g \times k_l}{(H/RT)k_g + k_l} \text{ cm / hr} \quad (7)$$

where:

- H = Henry's Law constant ($\text{atm}\cdot\text{m}^3/\text{mol}$)
- R = Universal gas constant ($8.2 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}\cdot\text{K}$)
- T = Temperature (K; $^{\circ}\text{C} + 273$)
- k_g = Gas-phase exchange coefficient
- k_l = Liquid-phase exchange coefficient.

The gas-phase exchange coefficient expression depends on the molecular weight (MW) of the compound. If MW is <65 g/mol, the following equation is used:

$$k_g = 3,000 \times (18/MW)^{1/2} \text{ cm / hr} \quad (8)$$

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

$$k_g = 1,137.5 \times (V_{wind} + V_{curr})(18/MW)^{1/2} \text{ cm / hr} \quad (9)$$

where:

$$\begin{aligned} V_{wind} &= \text{Wind velocity (m/sec)} \\ V_{curr} &= \text{Current velocity (m/sec)}. \end{aligned}$$

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:

$$k_1 = 20 \times (44/MW)^{1/2} \text{ cm / hr} \quad (10)$$

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

$$k_1 = 23.51 \times \left(V_{curr}^{0.969} / Z^{0.673} \right) \times (32/MW)^{1/2} \text{ cm / hr} \quad (11)$$

The following equation is used when V_{wind} is >1.9 m/sec and ≤ 5 m/sec, and MW is ≥ 65 g/mol:

$$k_1 = 23.51 \times \left(V_{curr}^{0.969} / Z^{0.673} \right) \times (32/MW)^{1/2} e^{0.526(V_{wind}-1.9)} \text{ cm / hr} \quad (12)$$

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

Combining Equations (6), (7), (8), and (10) into a single equation for estimating volatilization half-life ($\tau_{1/2}$) for compounds with MW <65 g/mol gives the following equation:

$$\tau_{1/2} = Z \times \ln 2 \times \left\{ \left[(1/20) \times (MW/44)^{1/2} \right] + \left[(RT/H \times 3000) \times (MW/18)^{1/2} \right] \right\} hr \quad (13)$$

The following equation, combining Equations (6), (7), (9), and (11), can be used to estimate the volatilization half-life ($\tau_{1/2}$) for compounds with MW \geq 65 g/mol if the wind velocity is \leq 1.9 m/sec:

$$\tau_{1/2} = Z \times \ln 2 \times \left\{ \left[(Z^{0.673}/23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2} \right] + \left[(RT/H \times 1,137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2} \right] \right\} hr \quad (14)$$

The following equation, combining Equations (6), (7), (9), and (12), can be used to estimate the volatilization half-life ($\tau_{1/2}$) for compounds with MW \geq 65 g/mol if the wind velocity is $>$ 1.9 m/sec and \leq 5 m/sec:

$$\tau_{1/2} = Z \times \ln 2 \times \left\{ \left[(Z^{0.673}/23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2} \right] e^{0.526(1.9-V_{wind})} + \left[(RT/H \times 1,137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2} \right] \right\} hr \quad (15)$$

If H is $<10^{-7}$ atm·m³/mol, the substance is less volatile than water and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, p. 15-15) and no volatilization half-life is estimated for rivers or lakes.

3.1.1 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 (13) and (15) reduce to the following:

$$MW < 65 \text{ g/mol}$$

$$\tau_{1/2} = 2.89 \times \left\{ \left[0.05 \times (MW/44)^{1/2} \right] + \left[(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2} \right] \right\} \text{days} \quad (16)$$

$$MW \geq 65 \text{ g/mol}$$

$$\tau_{1/2} = 2.89 \times \left\{ \left[0.185 \times (MW/32)^{1/2} \right] + \left[(3.6 \times 10^{-6}/H) \times (MW/18)^{1/2} \right] \right\} \text{days} \quad (17)$$

where:

$$\begin{aligned} H &= \text{Henry's Law constant (atm}\cdot\text{m}^3/\text{mol}) \\ MW &= \text{Molecular weight (g/mol)}. \end{aligned}$$

3.1.2 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 (13) and (14) reduce to the following:

- MW < 65 g/mol

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

- MW \geq 65 g/mol

$$\tau_{1/2} = 2.89 \times \left\{ \left[17.2 \times (MW/32)^{1/2} \right] + \left[(3.9 \times 10^{-6}/H) \times (MW/18)^{1/2} \right] \right\} \text{days} \quad (19)$$

where:

- H = Henry's Law constant (atm·m³/mol)
- MW = Molecular weight (g/mol).

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

In the evaluation of the ground water migration pathway, a hazardous substance that does not meet the criteria for an observed release is assigned a mobility factor value from HRS Table 3-8, *Ground Water Mobility Factor Values*, based on its soil water distribution coefficient (K_d) value and its water solubility value. K_d values that are not available in the references listed in Section 2.3.4, Soil Water Distribution Coefficient (K_d); Soil Organic/Carbon Partition Coefficients (K_{oc}), are calculated as detailed below:

HRS Section 3.2.1.2, *Mobility*, states:

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

Estimate K_d range for the hazardous substance using the following equation

$$K_d = (K_{oc})(f_s)$$

where:

K_{oc} = Soil-water partition coefficient for organic carbon for the hazardous substance.
 f_s = Sorbent content (fraction of clays plus organic carbon) in the subsurface

-- Use f_s values of 0.03 and 0.77 in the above equation to establish the upper and lower values of the K_d range for the hazardous substance.

-- Calculate the geometric mean of the upper and lower K_d range values. Use this geometric mean as the distribution coefficient in assigning the hazardous substance a mobility factor value from [HRS] Table 3-8.

SCDM uses the following references to calculate and to obtain K_d and K_{oc} values:

- U.S. EPA. 2001d. *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (Peer Review Draft). March. OSWER 9355.4-24.
- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document*. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502.
- Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.
- Di'Toro, D.M. 1985. A Particle Interaction Model of Reversible Organic Chemical Sorption. *Chemosphere*. 14(10):1503-1538.

Metals

For metals, SCDM uses K_d values contained in EPA's *Soil Screening Guidance* (EPA, 2001). These were estimated using the MINTEQA2 aqueous speciation geochemical model. When the required thermodynamic data were not available in the MINTEQA2 databases, the empirical pH-dependent relationships developed by the EPA ORD laboratory in Athens, Georgia, are used. SCDM contains values corresponding to typical subsurface pH (6.8).

Organic Substances

K_{oc} values for organic hazardous substances that ionize under subsurface pH conditions (i.e., pH=4.9 to 8.0) are derived by applying a theoretical relationship that accounts for both the neutral and the ionized fractions of the compound. Values corresponding to a typical subsurface pH (pH=6.8) are used in SCDM. The methodology used to develop these K_{oc} values is described in this reference as well.

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 semivolatile organic compounds:

$$\log K_{oc} = 0.00028 + (0.983 \log K_{ow}) \quad (20)$$

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):

$$\log K_{oc} = 0.00784 + (0.7919 \log K_{ow}) \quad (21)$$

3.3 Screening Concentration Benchmarks

The HRS assigns extra weight to targets with exposure to hazardous substances that are at or above benchmark values. In addition to the regulatory limits discussed in Section 2.8, Other Chemical Data, the HRS uses a number of benchmarks called screening concentrations. Screening concentrations correspond to a 10^{-6} individual cancer risk or a noncancer hazard quotient of 1 under specified exposure assumptions. The equations used for these estimations are taken from EPA's *Risk Assessment Guidance for Superfund (RAGS) Volume I, Part A* (EPA, 1989b) and *Part B* (EPA, 1991). The assumptions used in the calculations are conservative and broadly apply to sites nationwide. EPA recognizes that modeling human activity patterns would provide a more realistic determination of exposure or risk. While such information may be determined on a site-specific basis with considerable effort, it is difficult to develop assumptions on the activity patterns of target populations that could be applied to sites on a nationwide basis in order to develop exposure scenarios for the HRS. For this reason, the HRS exposure assumptions reflect values used for the assessment of risk throughout different programs within EPA. EPA recognizes that a critical evaluation of the references cited below, along with other information, could lead to differing exposure assumptions. Moreover, EPA continues to reassess assumptions used in this area of risk assessment. EPA also considered the limited number of samples available at the National Priority List (NPL) listing stage when it selected these assumptions. As outlined in the Field Test (54 FR 37949, September 14, 1989) of the revised HRS (40 FR Part 300, Final Rule, December 14, 1990), EPA generally expects to have <100 samples for all pathways to support the HRS analysis. This limited sampling may not include areas of maximum contamination, or "hot spots," and thus the sample results may not represent the maximum level of contamination. Although using conservative exposure assumptions does not fully compensate for the limited data available for analysis, using less conservative assumptions would likely lead to a greater incidence of false negatives (i.e., EPA may not identify sites that should be investigated further under the remedial program).

3.3.1 Screening Concentrations for Drinking Water Pathways

The following equation is used to calculate the average daily intake of a hazardous substance from the ingestion of contaminated ground water or surface water:

$$\text{AverageDailyIntake}(mg / kg - day) = \frac{C_{\text{water}} \times IR \times EF \times ED}{BW \times AT} \quad (22)$$

where:

- C_{water} = Contaminant concentration in water (mg/L)
- IR = Drinking water intake (ingestion) rate (L/day)
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)

BW = Body weight (kg)
 AT = Averaging time (days)

Under the assumption used for HRS purposes, the adult drinking water ingestion rate is 2 L/day, the exposure frequency for residents is daily (350 days/year), the exposure duration is 30 years, and the average adult body weight is 70 kg. The ingestion rate of 2 L/day is routinely used by EPA as the value for drinking water ingestion and assumes that the entire 2 L/day are from a contaminated drinking water source. Refinements in risk assessments sometime assume that an individual will be away for vacations or that some water will be consumed at the workplace.

Cancer Risk Screening Concentration

The cancer risk screening concentration is estimated by solving Equation (22) for the contaminant concentration in media of concern (C_{medium}), at a specific target risk level using the following relationship:

$$\text{Target Risk} = \text{Average Daily Intake} \times \text{Cancer Slope Factor (SF)} \quad (23)$$

When Equation (23) is rearranged to solve for the average daily intake (I), Equations (22) and (23) can be combined to estimate the water concentration (C_{water}) that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the drinking water screening concentration for carcinogens presumed to result in one excess case of cancer per million people exposed (i.e., 10^{-6} target risk level) (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times BW \times 25,550 \text{ days}}{SF_{\text{oral}} \times IR \times EF \times ED} \quad (24)$$

For non-radioactive carcinogens, Equation (24) can be simplified to:

$$SC_c (\text{mg} / \text{L}) = \frac{8.52 \times 10^{-5}}{SF_{\text{oral}}} \quad (25)$$

Because the cancer slope factors for radionuclides are in units of pCi^{-1} , body weight and averaging time do not apply. Some references, such as *HEAST* give a unique slope factor for each oral pathway (drinking water, food chain, and soil pathways). Thus, the following equation is analogous to Equation (24):

$$SC_c = \frac{10^{-6}}{SF_{oral(WATER,FOOD,orSOIL)} \times IR \times EF \times ED} \quad (26)$$

When the exposure assumptions described in Equation (22) are used, Equation (26) may be rewritten to estimate the concentration in water that corresponds to a target risk of 10^{-6} . The screening concentration for radionuclides ingested in water (SC_r) is given by:

$$SC_r(pC_i / L) = \frac{4.76 \times 10^{-11}}{SF_{oral(WATER)}} \quad (27)$$

Noncancer Risk Screening Concentrations

The RfD is based on the assumption that thresholds exist for certain toxic effects. In general, the RfD is an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. When the acceptable daily intake for drinking water ingestion is set equal to the RfD_{oral} (i.e., hazard quotient = 1), Equation (22) may be rearranged to solve for the contaminant concentration in water that corresponds to the no adverse effects level described above. To solve for the drinking water screening concentration for carcinogens (SC_n), Equation (22) becomes:

$$SC_n = \frac{RfD_{oral} \times BW \times AT}{IR \times EF \times ED} \quad (28)$$

For non-carcinogenic effects, the averaging time is 30 years or 10,950 days. When the assumptions in Equation (22) are used, Equation (28) can be simplified to:

$$SC_n(mg / L) = RfD_{oral} \times 36.5 \quad (29)$$

3.3.2 Screening Concentrations for the Surface Water Food Chain Pathway

The following equation is used to calculate the average daily intake from fish and shellfish ingestion (RAGS, EPA, 1989b):

$$\text{AverageDailyIntake}(\text{mg} / \text{kg} - \text{day}) = \frac{C_{\text{fish}} \times IR \times F \times EF \times ED}{BW \times AT} \quad (30)$$

where:

C_{fish}	=	Contaminant concentration in fish/shellfish (mg/kg)
IR	=	Fish/shellfish intake (ingestion) rate (kg/day)
F	=	Fraction ingestion from contamination sources (unitless)
EF	=	Exposure frequency (days/year)
ED	=	Exposure duration (years)
BW	=	Body weight (kg)
AT	=	Averaging time (days)

The high end ingestion rate for recreational fishers is 0.054 kg/day (USDA, 1982) with the fraction ingested (F) set to equal to 1 (i.e., all fish are assumed to come from contaminated waters). The exposure frequency is assumed to be 350 days/year, the exposure duration is 30 years, and the average adult body weight is 70 kg.

Cancer Risk Screening Concentration

When Equation (23) is rearranged to solve for the average daily intake (I), Equations (23) and (30) can be combined to estimate the fish/shellfish concentration that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the fish/shellfish concentration presumed to result in one excess case of cancer per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times BW \times 25,550 \text{ days}}{SF_{\text{oral}} \times IR \times F \times EF \times ED} \quad (31)$$

Using the exposure assumptions listed for Equation (30) results in a simplified screening concentration equation for non-radioactive carcinogenic substances in fish/shellfish:

$$SC_c(\text{mg/kg}) = \frac{3.15 \times 10^{-3}}{SF_{oral}} \quad (32)$$

If the same exposure assumptions are used, excluding body weight and averaging time, Equation (32) may be rewritten to estimate the fish/shellfish concentration that corresponds to a target risk level of 10^{-6} for ingestion of radionuclides in fish/shellfish (SC_r). Again, please note that some references such as *HEAST* give an oral slope factor to be used specifically for the food chain pathway:

$$SC_r(pCi/kg) = \frac{1.76 \times 10^{-9}}{SF_{oral(FOOD)}} \quad (33)$$

Noncancer Risk Screening Concentration

Setting the intake from fish and shellfish ingestion equal to the oral reference dose (RfD_{oral}) and solving Equation (30) for concentration gives the following equation:

$$SC_n = \frac{RfD_{oral} \times BW \times AT}{IR \times F \times EF \times ED} \quad (34)$$

For non-carcinogenic effects, the averaging time is 30 years, or 10,950 days. If the other assumptions listed for Equation (30) are used, Equation (34) may be simplified as follows:

$$SC_n(\text{mg/kg}) = RfD_{oral} \times 1,352 \quad (35)$$

3.3.3 Screening Concentrations for Soil Ingestion

The following equation is used to calculate the average daily intake from soil ingestion (RAGS, EPA, 1989b):

$$\text{AverageDailyIntake}(\text{mg} / \text{kg} - \text{day}) = \frac{C_{\text{soil}} \times CF \times IF \times EF}{AT} \quad (36)$$

where:

C_{soil}	=	Contaminant concentration in soil (mg/kg)
CF	=	Conversion factor (10^{-6} kg/mg)
IF	=	Age-adjusted soil ingestion factor (mg-yr/kg-day)
EF	=	Exposure frequency (days/year)
AT	=	Averaging time (days)

and IF is given by:

$$IF_{\text{soil/adj}}(\text{mg} - \text{yr} / \text{kg} - \text{day}) = \frac{IR_{\text{soil/age1-6}} \times ED_{\text{age1-6}}}{BW_{\text{age1-6}}} + \frac{IR_{\text{soil/age7-31}} \times ED_{\text{age7-31}}}{BW_{\text{age7-31}}} \quad (37)$$

where:

$IR_{\text{soil/age 1-6}}$	=	Soil intake (ingestion) rate, age 1 to 6 (mg/day)
$ED_{\text{age 1-6}}$	=	Exposure duration ages 1-6 (yr)
$BW_{\text{age1-6}}$	=	Average body weight from ages 1-6 (kg)

and

$IR_{\text{soil/age 7-31}}$	=	Soil intake (ingestion) rate, ages 7 and older (mg/kg)
$ED_{\text{age 7-31}}$	=	Exposure duration ages 7-31 (yr)
$BW_{\text{age7-31}}$	=	Average body weight from ages 7-31 (kg)

The soil ingestion rate is assumed to be 200 mg/day for ages 6 and younger, and 100 mg/day for ages 7 and older; the exposure durations are 6 years and 24 years for children and “adults” (ages 7 to 31), respectively; and the average body weights are 15 kg for children and 70 kg for adults. As with Equation (22), the exposure frequency is assumed to be 350 days/year. With these assumptions, the age-adjusted soil ingestion factor is 114 mg-yr/kg-day.

Cancer Risk Screening Concentration

By rearranging Equation (23) to solve for the average daily intake (I), Equations (23) and (36) can be combined to estimate the soil concentration that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an averaging time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the screening soil concentration presumed to result in one excess case per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times 25550 \text{days}}{SF_{oral} \times IR \times CF \times EF} \quad (38)$$

Using the assumptions in Equations (36) and (37) results in a simplified screening concentration equation for non-radioactive carcinogenic substances in soil:

$$SC_c (\text{mg/kg}) = \frac{0.640}{SF_{oral}} \quad (39)$$

Because cancer slope factors for radionuclides are provided in pCi^{-1} , body weight and averaging time do not apply. As a result, IF is calculated without body weight (BW) in Equation (37) and is equal to 3,600 mg-yr/day. When the other exposure assumptions described for chemical carcinogens are used, Equation (39) maybe rewritten to estimate the soil concentration that corresponds to a target risk level of 10^{-6} for ingestion of radionuclides in contaminated soils (SC_{cr}). Again, please note that some references such as *HEAST* give an oral slope factor to be used specifically for the food chain pathway:

$$SC_{cr} (\text{pCi/kg}) = \frac{7.94 \times 10^{-7}}{SF_{oral}(\text{SOIL})} \quad (40)$$

Noncancer Risk Screening Concentration

Setting the intake from soil ingestion equal to the oral reference dose (RfD_{oral}) and solving Equation (36) for concentration gives the following equation:

$$SC_n = \frac{RfD_{oral} \times BW \times AT}{IR \times CF \times EF \times ED} \quad (41)$$

For non-carcinogenic effects, the averaging time (AT) is a function of the exposure duration (ED) assumed for children of 6 years \times 365 days/year = 2,190 days. Assuming daily exposure (i.e., $EF = 350$ days/year), an average body weight of 15 kg, and an ingestion rate (IR) for children of 200 mg soil per day results in the following simplified equation:

$$SC_n(\text{mg} / \text{kg}) = RfD_{oral}(\text{mg} / \text{kg} - \text{day}) \times 78,214 \quad (42)$$

3.3.4 Screening Concentration for the Air Pathway

The following equation (*RAGS*, EPA, 1989b, p. 6-44) is used to calculate intake from inhalation of airborne hazardous substances:

$$\text{AverageDailyIntake}(\text{mg} / \text{kg} - \text{day}) = \frac{C_{air} \times IR \times EF \times ED}{BW \times AT} \quad (43)$$

where:

C_{air}	=	Contaminant concentration air (mg/m^3)
IR	=	Air intake (inhalation) rate (m^3/day)
EF	=	Exposure frequency (days/year)
ED	=	Exposure duration (years)
BW	=	Body weight (kg)
AT	=	Averaging time (days)

The inhalation rate is assumed to be 20 m^3/day , the exposure frequency is 350 days/year, the exposure duration is 30 years, and the average adult body weight is 70 kg.

Cancer Risk Screening Concentration

By rearranging Equation (23) to solve for the average daily intake (I), Equations (23) and (43) can be combined to estimate the concentration in air that corresponds to a 10^{-6} target risk level. Over a lifetime, the average daily intake may be calculated assuming an average time (AT) of 25,550 days (i.e., 70 years) for carcinogenic effects. Therefore, the air concentration presumed to result in one excess case of cancer per million people exposed (SC_c) is given by:

$$SC_c = \frac{10^{-6} \times BW \times 25550 \text{days}}{SF_{inhal} \times IR \times EF \times ED} \quad (44)$$

Using the exposure assumptions listed above for Equation (43) results in the following equation for non-radioactive carcinogenic substances:

$$SC_c (\text{mg}/\text{m}^3) = \frac{8.52 \times 10^{-6}}{SF_{inhal}} \quad (45)$$

Using the same exposure assumptions (excluding body weight and averaging time), Equation (44) may be rewritten to estimate the air concentration of radionuclides that corresponds to a target risk level of 10^{-6} for inhalation of contaminated air (SC_r):

$$SC_r (\text{pCi}/\text{m}^3) = \frac{4.76 \times 10^{-12}}{SF_{inhal}} \quad (46)$$

Noncancer Risk Screening Concentration

Setting the average daily intake to the inhalation reference dose (RfD_{inhal}) and solving Equation (44) for the air concentration results in the following equation:

$$SC_n = \frac{RfD_{inhal} \times BW \times AT}{IR \times EF \times ED} \quad (47)$$

For non-carcinogenic effects, the averaging time (AT) is 30 years, or 10,950 days. The inhalation rate (IR) is assumed to be 20 m³/day; the exposure frequency (EF) is 350 days/year; the exposure duration (ED) is 30 years; and the average adult body weight (BW) is 70 kg. When these assumptions are used, Equation (47) maybe simplified as:

$$SC_n (mg / m^3) = RfD_{inhal} \times 3.65 \quad (48)$$

4.0 CHEMICAL DATA, FACTOR VALUES, AND BENCHMARKS

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

Figure 1 presents the header that appears on both sides of the page report. The header contains the date the report was printed, the substance name and synonym, the SCDM version (month, year), and the Chemical Abstract Service (CAS) number for the substance.

SUPERFUND CHEMICAL DATA MATRIX		
Date: 1/12/2004	Chemical: Acenaphthene	CAS Number: 000083-32-9
Figure 1. Page Heading		

The first page contains all of the selected chemical data, the data units, and an acronym describing the source of the information in SCDM. The chemical data are divided into six functional groups: toxicity, persistence, physical characteristics, mobility, bioaccumulation, and other data.

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

TOXICITY			
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Source</u>
Oral RfD:	6.00E-02	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	5.00E+02	µg/L	ECOTOX
Salt Ecol LC50:	1.70E+02	µg/L	ECOTOX
Figure 2. Toxicity Section			

The top half of this section contains the data used to determine the human toxicity factor value: reference dose (oral and inhalation), cancer slope factor (oral and inhalation), ED₁₀ (oral and inhalation), LD₅₀ (oral and dermal), and LC₅₀ (gas and dust inhalation). The bottom half of this section contains the data used to determine an ecotoxicity factor value: acute and chronic water quality criteria, Criteria Maximum Concentration (CMC) and Criteria Continuous Concentration (CCC), for fresh and salt water as well as fresh and salt water LC₅₀ values. Blank entries indicate that no value was found using the procedures and references specified in Section 2.2, Toxicity Information.

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

PERSISTENCE			
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Source</u>
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.1E+2	days	THOMAS
Photolysis:	2.5E+0	days	FATERATE
Biodeg:	1.0E+2	days	FATERATE
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.3E+0	days	THOMAS
Photolysis:	2.5E+0	days	FATERATE
Biodeg:	1.0E+2	days	FATERATE
Radio:		days	
Log Kow:	3.9E+0		CHEMFATE

Figure 3. Persistence Section

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

PHYSICAL CHARACTERISTICS	
<u>Parameter</u>	<u>Value</u>
Metal Contain:	No
Organic:	Yes
Gas:	Yes
Particulate:	Yes
Radionuclide:	No
Rad. Element:	No
Molecular Weight:	1.5E+2
Density:	1.2E+0 g/mL @ 20.00 C

Figure 4. Physical Characteristics Section

The mobility section (Figure 5) contains the air and ground water mobility data compiled using the methodology described in Section 2.3, Mobility Information. Vapor pressure and Henry's Law constant are used to determine gas migration potential and gas mobility factors. Henry's Law constant 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 nonmetalloid substances, whereas for metal-containing substances, the solubility value is the geometric mean of the available water solubilities for inorganic compounds containing the hazardous substance.

MOBILITY			
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Source</u>
Vapor Press:	2.5E-3	Torr	CHEMFATE
Henry's Law:	1.6E-4	atm-m ³ /mol	CHEMFATE
Water Solub:	3.6E+0	mg/L	CHEMFATE
Distrib Coef:	1.1E+9	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

Figure 5. Mobility Section

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

BIOACCUMULATION			
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Source</u>
FOOD CHAIN			
Fresh BCF:	387.00		VER_BCF
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:	387.00		VER_BCF
Salt BCF:			
Log Kow:	3.9E+0		CHEMFATE
Water Solub:	3.6E+0		CHEMFATE

Figure 6. Bioaccumulation Section

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

OTHER DATA	
Melting Point: 9.3E+1	C
Boiling Point: 2.8E+2	C
Formula: C ₁₂ H ₁₀	

Figure 7. Other Data

The class information section (Figure 8) lists parent substances for three data substitution classes: toxicity, ground water mobility, and other data. The toxicity class includes all toxicity and benchmark data used to determine human or ecotoxicity factor values. The ground water mobility class includes water solubility, soil/water distribution coefficient, and geometric mean water solubility. The “other” class includes hydrolysis, biodegradation, photolysis, and volatilization half-lives, as well as BCFs and Log K_{ow} . This section may also list other class-parent chemical substitutions for specific data elements.

Currently, only two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for the ground water mobility class with the elemental metal as the class parent. Radioactive isotopes may inherit data from their primary radioactive element for the ground water mobility and “other” classes.

CLASS INFORMATION	
<u>Class</u>	<u>Parent Substance</u>

Figure 8. Class Information Section

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

ASSIGNED FACTOR VALUES					
AIR PATHWAY		GROUND WATER PATHWAY		SOIL EXPOSURE PATHWAY	
<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>
Toxicity:	10	Toxicity:	10	Toxicity:	10
Gas Mobility:	0.2000	Water Solub:	3.6E+0		
Gas Migration:	11	Distrib:	1.1E+9		
		Geo Mean Sol:			
		Liquid Karst:	1.0E+0		
		Non Karst:	1.0E-4		
		Non Liq. Karst:	2.0E-1		
		Non Karst:	2.0E-5		
SURFACE WATER PATHWAY					
DRINKING WATER		HUMAN FOOD CHAIN		ENVIRONMENTAL	
<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>
Toxicity:	10	Toxicity:	10	Fresh Tox:	10000
				Salt Tox:	1000
Persistence		Persistence		Persistence	
River:	0.4000	River:	0.4000	River:	0.4000
Lake:	0.4000	Lake:	0.4000	Lake:	0.4000
		Bioaccumulation		Bioaccumulation	
		Fresh:	500.0	Fresh:	500.0
		Salt:	500.0	Salt:	500.0

Figure 9. Assigned Factor Values Section

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

BENCHMARKS											
AIR PATHWAY			GROUND WATER PATHWAY			SOIL EXPOSURE PATHWAY			RADIONUCLIDE		
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Parameter</u>	<u>Value</u>	<u>Unit</u>
NAAQS/NESHAPS:		µg/m3	MCL/MCLG:		mg/L	Cancer Risk:		mg/kg	MCL:		pCi/L
Cancer Risk:		mg/m3	Cancer Risk:		mg/L	Non Cancer Risk:	4.7E+3	mg/kg	UMTRCA:		pCi/kg
Non Cancer Risk:		mg/m3	Non Cancer Risk:	2.2E+0	mg/L				CANCER RISK		
									Air:		pCi/m3
									DW:		pCi/L
									FC:		pCi/kg
									Soil Ing:		pCi/kg
									Soil		pCi/kg
									Gam:		
SURFACE WATER PATHWAY											
DRINKING WATER			HUMAN FOOD CHAIN			ENVIRONMENTAL					
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Parameter</u>	<u>Value</u>	<u>Unit</u>			
MCL/MCLG:		mg/L	FDAAL:		ppm	ACUTE					
Cancer Risk:		mg/L	Cancer Risk:		mg/kg	Fresh CMC:		µg/L			
Non Cancer Risk:	2.2E+0	mg/L	Non Cancer Risk:	8.1E+1	mg/kg	Salt CMC:		µg/L			
Risk:			Risk:								
						CHRONIC					
						Fresh CCC:		µg/L			
						Salt CCC:		µg/L			

Figure 10. Benchmarks Section

Appendix B contains tables for both radioactive and nonradioactive hazardous substances. Appendix B is divided into two sections, Appendix B-I and B-II. Appendix B-I contains all of the factor values by pathway, including radionuclides. Appendix B-II presents all the benchmarks by pathway, including radionuclides. Appendix C contains a cross-reference index of hazardous substance names, synonyms, and CAS numbers for substances in SCDM.

5.0 REFERENCES

- American Conference of Governmental Industrial Hygienists (ACGIH). 2001. *Documentation of the Threshold Limit Value and Biological Exposure Indices*. 7th Edition. ACGIH, Cincinnati, OH.
- Baes, C.F., III, R.D. Sharp, and A.L. Sjoreen, and R.W. Shor. 1984. *A Review and Analysis of Parameters for Assessing Transportation of Environmentally Released Radionuclides through Agriculture*. Oak Ridge National Laboratory, TN. ORNL-5786.
- C-E Environmental, Inc. 1990. *The Identification of Health Effects Data for Chemicals Contained in the Clean Air Act Amendments: Final Report to Dr. John Vanderburg*. U.S. Environmental Protection Agency, Research Triangle Park, NC.
- 40 CFR Part 50. 2001. National Ambient Air Quality Standards. November.
- 40 CFR Part 61. 1994. National Emissions Standards for Hazardous Air Pollutants.
- 40 CFR Part 192. 1994. Uranium Mill Tailings Radiation Control Act Standards.
- Dean, J.A. (Ed.). 2002. *Lange's Handbook of Chemistry*, 15th Edition. McGraw-Hill, New York.
- Di'Toro, D.M. 1985. A particle Interaction Model of Reversible Organic Chemical Sorption. *Chemosphere*. 14(10):1503-1538.
- 55 FR 51583-51667. *Hazard Ranking System, Final Rule*. 14 December 1990.
- Howard, Philip H., W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. *Handbook of Environmental Degradation Rates. (FATERATE)* Lewis Publishers, In. Chelsea, Michigan.
- International Commission on Radiological Protection (ICRP). 1983. *Radionuclide Transformations: Energy and Intensity of Emissions*. ICRP Publication No. 38. Pergamon Press, New York.
- Lide, D.R. (Ed.). 2002-2003. *CRC Handbook of Chemistry and Physics*, 83rd Edition. CRC Press, Boca Raton, FL.
- Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society, Washington, DC.
- National Institute for Occupational Safety and Health (NIOSH). 2002. *Registry of Toxic Effects of Chemical Substances (RTECS)*. Accessed October 2003. (<http://grc.ntis.gov>).
- O'neil, M., and A. Smith (Eds). 2001. *The Merck Index*, 13th Edition. Merck & Co., Inc., Rahway, NJ.
- Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

- Syracuse Research Corporation (SRC). 2003a. *CHEMFATE Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/efdb/chemfate.htm>).
- Syracuse Research Corporation (SRC). 2003b. *PHYSPROP Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/interkow/physdemo.htm>).
- Thomas, R.G. 1990. "Volatilization from Water." In *Handbook of Chemical Property Estimation Methods*. W.J. Lyman, W.F. Reehl, D.H. Rosenblatt, Eds. American Chemical Society, Washington, DC. pp. 15-9-15-28.
- U.S. Environmental Protection Agency (EPA). 1986. *Superfund Public Health Evaluation Manual (SPHEM)*. Exhibit A-1: Physical, Chemical, and Fate Data. Office of Emergency and Remedial Response, Washington, DC (EPA/540/1-86/060)(OSWER Directive 9285.4-1).
- U.S. EPA. 1988. *Methodology for Evaluating Potential Carcinogenicity in Support of Reportable Quantity Adjustments Pursuant to CERCLA Section 102*. Office of Health and Environmental Assessment, Washington, DC (EPA/600/8-89/053).
- U.S. EPA. 1989a. *Interim Procedures for Estimating Risks Associated with Mixtures of Chlorinated Dibenzo-p-Dioxins and Dibenzofurans (CDDs and CDFs) and 1989 Update*. Risk Assessment Forum, Washington, DC (EPA/625/3-89-016).
- U.S. EPA. 1989b. *Risk Assessment Guidance for Superfund (RAGS): Volume 1- Human Health Evaluation Manual. Part A. Interim Final*. Office of Emergency and Remedial Response, Washington, DC. (EPA/540/1-89/002).
- U.S. EPA. 1991. *Risk Assessment Guidance for Superfund (RAGS): Volume I- Human Health Evaluation Manual (Part B, Development of Risk-Based Preliminary Remediation Goals). Interim*. Publication 9285.7-01B. Office of Emergency and Remedial Response, Washington, DC. NTIS PB92-963333.
- U.S. EPA. 1994. *Estimating Exposure to Dioxin Like Compounds* (EPA/600/6-88/005Ca). June.
- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document*. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, D.C. NTIS PB96-963502. Accessed October 2003. (<http://www.epa.gov/superfund/resources/soil/index.htm>).
- U.S. EPA. 1999. *Guidelines for Carcinogenic Risk Assessment*. Review Draft. July.
- U.S. EPA. 2000a. EPA's PCB Risk Assessment Review Guidance Document, Interim Draft. January.
- U.S. EPA. 2000b. Part III: *Integrated Summary and Risk Characterization for 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds*. Office of Research and Development, National Center for Environmental Assessment. June. (EPA/600/P-00/Ag).
- U.S. EPA. 2000c. *Chapter 9: Toxicity Equivalence Factors (TEFs) for Dioxin and Related Compounds*. Office of Research and Development, National Center for Environmental Assessment. June.

- U.S. EPA. 2000d. *Exposure and Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds*. Office of Research and Development, National Center for Environmental Assessment. (EPA/600/P-00/001Ab-Ae). March/May.
- U.S. EPA. 2000e. *Soil Screening Guidance for Radionuclides: User's Guide* (EPA/540-R-00-007, PB2000 963307). Accessed October 2003. (<http://www.epa.gov/superfund/resources/radiation/radssg.htm>).
- U.S. EPA. 2001a. *Superfund Technical Support Center Provisional Toxicity Issue Papers (STSCPVT)*. Office of Research and Development, Washington, DC. February. Accessed November 2003. (<http://epa-heast.ornl.gov/provinsional.html>).
- U.S. EPA. 2001b. *Health Effects Assessment Summary Tables (HEAST): Summary of HEAST Values*. Office of Radiation and Indoor Air, Washington, DC. February. Accessed November 2003. (<http://epa-heast.ornl.gov>).
- U.S. EPA. 2001c. *HEAST Radionuclide Table: Carcinogenicity - Slope Factors*. Office of Radiation and Indoor Air, Washington, DC. April. Accessed November 2003. (<http://www.epa.gov/radiation/heast/index.html>).
- U.S. EPA. 2001d. *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (Peer Review Draft), OSWER 9355.4-24. March. (<http://www.epa.gov/superfund/resources/soil/index.htm>).
- U.S. EPA. 2002. *National Recommended Water Quality Criteria - 2002*. Office of Water. Washington, DC. November.
- U.S. EPA. 2003a. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. Accessed November 2003. (<http://www.epa.gov/iris>).
- U.S. EPA. 2003b. *ECOTOX Database*. Environmental Research Laboratory, Duluth, MN. Accessed December 2003. (<http://www.epa.gov/ecotox>).
- U.S. EPA. 2003c. *National Primary Drinking Water Standards*. Accessed through *List of Drinking Water Contaminants and MCLs*. Office of Water, Washington, DC. (<http://www.epa.gov/safewater/mcl.html>).
- U.S. Food and Drug Administration. 2000. *Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed*. Center for Food Safety and Applied Nutrition, Washington, DC. Accessed September 2003. (<http://www.cfsan.fda.gov/~lrd/fdaact.html>).
- Versar, Inc. 1990. *Issue Paper: Bioaccumulation Potential Based on Ambient Water Quality Criteria Documents*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC. Contract No. 68-W8-0098.