APPENDIX E

BACKGROUND INFORMATION FOR THE DEVELOPMENT OF REFERENCE GROUND-WATER CONCENTRATION VALUES

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BACKGROUND INFORMATION FOR THE DEVELOPMENT OF REFERENCE GROUND-WATER CONCENTRATION VALUES

E-1 Shower Model

E-1.1 Shower Model

The shower model calculates the incremental change in the concentration of a constituent in air that results from the transfer of constituent mass from the water phase (the shower water) to the vapor phase (the air in the shower stall) over time. The model then estimates the concentration of the constituent in a bathroom that results from air exchange within the bathroom and between the bathroom and the rest of the house over time. After the model calculates the predicted air-phase constituent concentration in the shower stall and bathroom, we use those concentrations to estimate the average air-phase constituent concentration to which an individual is exposed over the course of an entire day. We use this average daily concentration to calculate inhalation HBNs.

The shower model is based on differential equations presented in McKone (1987) and Little (1992a). We solved the differential equations using a mathematical technique called “finite difference numerical integration,” to produce the equations that we use in our analysis, Equations E-1 to E-11 in this Appendix. In reviewing the equations and reading the following sections, it will help to keep in mind the following two concepts:

> *We calculate air-phase constituent concentrations for different “compartments*.” The shower model is based on the understanding that there are two compartments in the bathroom: 1) the shower stall and 2) the rest of the bathroom (outside of the shower stall). We assume that an adult spends time: in the shower stall when the shower is running; in the shower stall after the shower is turned off; and in the rest of the bathroom after the shower is turned off (see Equations E-1 and E-2).
>
> *We calculate air-phase constituent concentrations for different time steps*. We implement the shower model in time steps. That is, we estimate the air-phase constituent concentration in each of the two compartments in 0.2-minute increments or time steps. The air-phase constituent concentration at the beginning of the 0.2-minute time step differs from the concentration at the end of the 0.2-minute time step because of volatilization of constituent mass from the shower water (which adds constituent mass) and the exchange of air between the compartments in the bathroom and the rest of the house (which disperses the mass). At the beginning of a time step, the air-phase concentration in each

bathroom compartment is equal to the air-phase concentration that was estimated for the compartment at the end of the previous time step.

The following is our basic procedure for implementing the shower model:

- Calculate a mass transfer coefficient for each constituent;
- Estimate the air-phase constituent concentration in the shower stall for sequential 0.2-minute time steps;
- Estimate the air-phase constituent concentration in the bathroom (other than in the shower stall) for sequential 0.2-minute time steps;
- Use the air-phase constituent concentrations calculated for the shower stall, and the air-phase constituent concentrations calculated for the bathroom, to calculate the average constituent concentration to which an adult is exposed during the course of a day.

This procedure is explained in greater detail below. Table E-2 provides the values for the constituent-specific properties used in the model. Table E-1 provides the values we used for the parameters in the model.

Calculating a Mass Transfer Coefficient

The first step in estimating the concentration of a constituent in air is to quantify the constituent's "resistance" to movement between the water phase and the air phase. We quantify this resistance using the mass transfer coefficient presented in Equation E-4, which incorporates variables calculated in Equations E-3 and E-5. The mass transfer coefficient depends on properties specific to each constituent evaluated, as well as physical properties of the water droplet. Specifically, the mass transfer coefficient depends on:

- The constituent's diffusivity in water (the molecular diffusion coefficient for the constituent in water), which determines how readily the constituent mass in the center of the water droplet will diffuse to the surface of the water droplet. If a constituent's diffusivity in water is low, then as the constituent is emitted from the surface of the water droplet, the rate at which the surface of the droplet is "supplied" with constituent from the center of the water droplet will be slow, resulting in less constituent being emitted from the droplet. Diffusivity influences the concentration gradient across the droplet.

- The Henry's law constant for the constituent, which establishes how the constituent will partition between the water phase and the air phase to achieve equilibrium. Henry's law states that, at equilibrium, the amount of a constituent dissolved in water is proportional to the amount of the constituent in the air phase that is in contact with the water. This proportion is constituent-specific (each constituent has a different Henry's law constant). The Henry's law constant influences the magnitude of the air-phase constituent concentrations more than any other constituent-specific parameter.

- The constituent's diffusivity in air (the molecular diffusion coefficient for the constituent in air), which determines how readily the constituent will migrate away from the droplet once it is released into the air surrounding the droplet. Constituents with lower diffusivities in air will have comparatively higher concentrations around the water droplet than in the surrounding air. Therefore, because of Henry's law, less constituent would need to come out of solution into the air phase in order to achieve equilibrium.

- The amount of time that the droplet is in contact with the air, which we assume is equivalent to the time it takes for the droplet to fall to the floor of the shower. We determine the time it takes the droplet to fall by dividing distance that the droplet has to fall (which we assume is equal to the height of the shower nozzle) by the velocity at which the water droplet falls (which we assume is the terminal velocity of the droplet). For this analysis, we set the nozzle height and the terminal velocity of the droplet at fixed values, as presented in Table E-1.

- The ratio of the water droplet's surface area to its volume. Because we assume that the droplet is a sphere, its surface area to volume ratio is equal to a value of 6 divided by the diameter of the droplet. For this analysis, the diameter of the droplet, therefore its surface area to volume ratio, is a fixed value (see Table E-1).

Table E-2 presents the constituent-specific diffusivities and Henry's law constants that we used in our analysis.

Table E-1. Shower Model Input Parameters

Input Parameter	Description	Value	Units	Reference	Comment
Bathroom Properties					
Vb	Volume of the bathroom	10	m^3	McKone, 1987	
Exchange Rate					
Qbh	Volumetric exchange rate between the bathroom and the house	300	L/min	derived value	Estimated from the volume and flow rate in McKone (1987) such that the exchange rate equals the volume divided by the residence time (e.g., 10,000L/30 min).
Qsb	Volumetric exchange rate between the shower and the bathroom	100	L/min	derived value	Estimated from the volume and flow rate in McKone (1987) such that the exchange rate equals the volume divided by the residence time (e.g., 2000L/20 min).
Exposure Time					
ShowerStallTime	Time in shower stall after showering	5	min	U.S. EPA, 1997c	Table 15-23. 50th percentile overall
T_bathroom	Time spent in bathroom, not in shower	5	min	U.S. EPA, 1997c	Table 15-32. 50th percentile overall
ShowerTime	Shower time, 50th percentile	15	min	U.S. EPA, 1997c	Table 15-21. 50th percentile overall
Shower Properties					
Vs	Volume of shower	2	m^3	McKone, 1987	
NozHeight	Height of shower head	1.8	m	Little, 1992a	Selected based on the maximum height reported in Table 1 of Little (1992a), a summary of five studies.
ShowerRate	Rate of water flow from shower head	10	L/min	derived value	Value obtained by averaging the flow rates reported in five studies in Table 1 of Little (1992a) (QL) = 10.08 L/min.
DropVel	Terminal velocity of water drop	400	cm/s	derived value	Selected value by correlating to existing data.
DropDiam	Diameter of shower water drop	0.098	cm	derived value	Estimated as a function of terminal velocity<=600cm/sec (Coburn, 1996).
Groundwater					
Cin	Constituent concentration in incoming water	0.001	mg/L	NA	Unit concentration selected.

Calculating the Air-Phase Constituent Concentration in the Shower

Calculating the air-phase constituent concentration in the shower at the end of each time step involves:

1. Calculating the fraction of constituent that can be emitted into the air from each water droplet (Equation E-7);

2. Translating the fraction of constituent that can be emitted from each water droplet (from step 1) into the mass of constituent that is emitted from the entire volume of water that is coming into the shower during each time step (Equation E-6); and

3. Determining the constituent concentration at the end of the time step by: calculating the concentration added to the shower air during the time step (dividing the constituent mass emitted from the water in step 2 by the volume of the shower); adding this concentration to the concentration of the constituent that was already in the shower air at the beginning of the time step; and subtracting the concentration lost from the shower air due to the exchange of air with the rest of the bathroom (Equation E-9).

An important element of this analysis is the difference between the time in the shower stall that is spent showering (15 minutes, Table E.1) and the time in the shower stall that occurs after showering (5 minutes, Table E.1). The difference in these two time periods involves how we handle the value for mass of constituent emitted from the shower water (step 2, above). When we switch the model over from the time period where the shower nozzle is turned on (the time spent showering), to the time period where the shower nozzle is turned off (the time spent in the shower stall after showering), we set the mass emitted from the water to zero. This means that during the 5-minute period when the individual is in the shower after the shower is turned off, the air-phase concentration of the constituent is only a function of the concentration of the constituent in the air at the beginning of the time step and the air exchange between the shower stall and the rest of the bathroom. The following paragraphs describe steps 1 and 2 in more detail.

The fraction of the constituent mass that potentially can be emitted from a droplet at any given time during the droplet's fall through the air (Equation E-7) is a function of the mass transfer coefficient (the constituent's resistance to movement from the water phase to the air phase, described previously) and the "fraction of gas phase saturation" in the shower (calculated using Equation E-8). Inherent in this calculation is an assumption that the concentration of the constituent in the air is constant over the time it takes the droplet to fall. The fraction of gas phase saturation is an expression of how close the air-phase constituent concentration is to the maximum possible (equilibrium) air-phase concentration. Stated another way, Henry's law dictates that for a certain constituent concentration in water, we can predict the maximum concentration of constituent in the air that is in contact with the water (assuming the air and water are in equilibrium). Consequently, if there is already constituent in the air, then, to maintain equilibrium, there is a limit to how much additional constituent can be emitted from the water to the air (the less constituent already present in the air, the more constituent that theoretically may be emitted). The fraction of gas phase saturation is an expression of how close the air concentration is to that limit at the beginning of each time step. However, as suggested at the beginning of this paragraph, even though Henry's law influences the maximum fraction of mass that could be emitted from the droplet, the mass transfer coefficient also influences how much of the constituent will "free itself" from the water. Factors such as the constituent's dispersivity (in water and air) and the surface area of the droplet also influence the fraction of constituent mass that can be emitted from the droplet.

In most cases, for each 0.2-minute time step we evaluate, the mass of a constituent emitted from the shower water to the air is the product of: the concentration of the constituent in the shower water; the volume of water emitted from the shower during the time step; and the fraction of the constituent mass in the water that potentially could be emitted from the water (discussed above). However, in certain cases (typically rare), the mass transfer coefficient is of a magnitude that the concentration calculated in this way exceeds the mass that possibly could be emitted when the water and the air phases are at equilibrium. In this case, we "cap" the constituent mass that can be emitted from the shower water during the time step. The cap is the maximum constituent mass that could be emitted from the water at equilibrium (based on Henry's law) minus the constituent mass already in the shower stall at the beginning of the time step

Calculating the Air-Phase Constituent Concentration in the Bathroom (other than in the Shower Stall)

The air-phase constituent concentration in the bathroom (Equation E-10) is a function of the air-phase constituent concentration calculated for the shower, and the exchange of air 1) between the shower and the bathroom and 2) between the bathroom and the rest of the house. Specifically, for each time step, the air-phase constituent concentration in the bathroom is equal to: the air-phase constituent concentration in the bathroom at the beginning of the time step, plus the constituent concentration added as a result of the exchange of air with the shower, minus the constituent concentration lost as a result of the exchange of air with the rest of the house. Table E-1 presents the values we used for the volumetric exchange rate between the shower and the bathroom; the volumetric exchange rate between the bathroom and the house; and the volume of the bathroom.

Calculating the Average Daily Constituent Concentration to which an Individual is Exposed

To calculate the average concentration of a constituent to which an individual is exposed on a daily basis (24 hours per day) (Equation E-11), we:

1. Calculate the average constituent concentration in the shower air across all time steps and multiply this concentration by the amount of time an individual spends in the shower stall (Equation E-2);
2. Calculate the average constituent concentration in the bathroom air (not including the shower air) across all time steps and multiply this concentration by the amount of time an individual spends in the bathroom (not including the time spent in the shower stall);
3. Sum the values calculated in steps 1 and 2, and divide the sum by the length of a day. This calculation carries with it an assumption that an individual only is exposed to the constituent in the shower, and in the bathroom after showering (that is, that the concentration of the constituent in the rest of the house is zero).

E-1.2 Shower Model Uncertainties and Limitations

The primary limitations and uncertainties of the shower model are as follows:

- The model is constructed such that air-phase concentration of a constituent in household air results solely from showering activity. Individuals are exposed to emissions via inhalation for time spent in the shower while showering, in the shower stall after showering, and in the bathroom after showering. Other models calculate indoor air concentrations resulting from emissions from household use of tap water and/or calculate inhalation exposures for time spent in the remainder of the house. However, McKone (1987) found that the risk from inhalation exposures in the remainder of the house was considerably lower than the risk from inhalation exposures in the bathroom and during showering. In addition, there are few data available to estimate the input parameters needed to calculate exposure concentrations from other household activities, including variables such as house volume, air exchange rate between the house and outside air, and exposure time in the house. Given the expected lower risk due to exposure in the remainder of the house, and the lack of available data to estimate house constituent concentrations, we focused on showering as the greatest source of inhalation exposure and risk due to use of contaminated water.

- The model currently only considers exposures to adults who shower, and does not consider exposures to children who bathe in bathtubs. This limitation of the model may be significant. A recent report by EPA's National Center for Environmental Assessment states that: "Because of the longer exposure times, chemical emissions during the use of bathtubs may be as, or more, significant than during showers, in terms of human inhalation. This is particularly important given that small children are typically washed in bathtubs rather than showers and are generally more sensitive to chemical exposure than are healthy adults" (U.S. EPA, 2000).

- Our analysis does not consider an individual's dermal exposure to water or an individual's incidental ingestion of water while showering.

- The model only considers emissions that result from falling droplets of water in the shower. The model does not include algorithms that account for emissions from water films on shower walls or puddles on the floor of the shower. Use of the model also assumes that a droplet falls directly from the shower nozzle to the shower stall floor, and is not intercepted by the body of the individual who is showering.

- The input parameter values are a source of uncertainty for the shower model. To select values for the shower properties (shower and bathroom volume, nozzle height, and flow rate), we generally used central tendency values that were reported in the literature. Although fixing shower model input parameters as constant does not capture variability in the results, the results still compare favorably to experimental data for numerous organic compounds of varying volatility (Coburn, 1996). The values for droplet properties (diameter and velocity) are also constants, and are based on correlation to existing data. The largest uncertainty is likely in the volumetric exchange rates used between the shower and bathroom and the bathroom and the rest of house. We derived these values, 300 L/min for the exchange rate between the bathroom and house, and 100 L/min for the exchange rate between the shower and bathroom, from McKone (1987). However, values reported in a five-study summary by Little (1992a) ranged from 35 to 460 L/min for the exchange between the shower and bathroom, and 38 to 480 L/min for the exchange between the bathroom and the rest of the house. Such a large range of volumetric exchange rates imparts uncertainty to the shower model's estimation of constituent concentrations.

- A constituent's solubility in water depends on a number of factors including the temperature of the water and the other chemicals (for example, other solvents) that are in the water. When the concentration of a constituent in water exceeds the constituent's solubility in that water, we expect that at least some of the constituent will exist in the water as a non-aqueous (free) phase. Henry's law, a basic principle of the shower model, only applies to constituents dissolved in water, it does not apply to non-aqueous phase constituents (U.S. EPA, 1996). As a result, it would not be appropriate to use the HBNs we developed for the inhalation pathway if the shower water (which we assume is from a ground-water well) contained non-aqueous phase constituent. More importantly, however, EPACMTP, the ground-water fate and transport model that we use to estimate constituent concentrations in the modeled ground water, cannot be used to model non-aqueous phase liquids. Consequently, the IWEM tool should not be used in cases where non-aqueous phase constituents are present in leachate. In these situations, another tool must be used that is capable of evaluating non-aqueous phase liquids.

Equation E-1. Total time spent in shower and bathroom

$$BSResTime = ShowerTime + ShowerStallTime + T\_bathroom$$

Name	Description	Value
BSResTime	Total time spent in shower and bathroom (min)	Calculated above
ShowerTime	Duration of shower (min)	Provided in Table E-1
ShowerStallTime	Time in shower stall after showering (min)	Provided in Table E-1
T_bathroom	Time spent in bathroom, not in shower (min)	Provided in Table E-1

This equation calculates the total time that a receptor is exposed to vapors.

Equation E-2. Total time spent in shower stall

$$ShowerResTime = ShowerStallTime + ShowerTime$$

Name	Description	Value
ShowerResTime	Total time spent in shower stall (min)	Calculated above
ShowerStallTime	Time in shower stall after showering (min)	Provided in Table E-1
ShowerTime	Duration of shower (min)	Provided in Table E-1

This equation calculates the total time that a receptor is exposed to vapors in the shower stall.

Equation E-3. Dimensionless Henry's law constant

$$Hprime = HLCcoef \times HLC$$

$$HLCcoef = \frac{1}{R \times Temp}$$

Name	Description	Value
H*prime*	Dimensionless Henry's law constant (dimensionless)	Calculated above
HLCcoef	Coefficient to Henry's law constant Mol/(atm-m^3)	Calculated above
HLC	Henry's law constant (atm-m^3/Mol)	Chemical-specific
R	Ideal Gas constant (atm-m^3/K-Mol)	0.00008206
Temp	Temperature (K)	298

This equation calculates the dimensionless form of Henry's law constant.

Equation E-4. Dimensionless overall mass transfer coefficient

$$\mathrm{N} = \mathrm{Kol} \times \mathrm{AVRatio} \times \mathrm{DropResTime}$$

$$AVRatio = \frac{6}{DropDiam}$$

$$\mathrm{DropResTime} = \frac{NozHeight \times 100}{DropVel}$$

Name	Description	Value
N	Dimensionless overall mass transfer coefficient (dimensionless)	Calculated above
AVRatio	Area-to-volume ratio for a sphere (cm^2/cm^3)	Calculated above
Kol	Overall mass transfer coefficient (cm/s)	Calculated in Equation E-5
DropResTime	Residence time for falling drops (s)	Calculated above
DropDiam	Drop diameter (cm)	Provided in Table E-1
NozHeight	Nozzle height (m)	Provided in Table E-1
DropVel	Drop terminal velocity (cm/s)	Provided in Table E-1
100	Conversion factor (cm/m)	Conversion factor

This equation calculates the dimensionless overall mass transfer coefficient. The above equation is based on Little (1992a; Equation 5), which provides the equation as N = Kol × A/Q1 where A is the total surface area for mass transfer and Q1 is water flow in volume per time.

Equation E-5. Overall mass transfer coefficient

$$Kol = \beta \times \left(\frac{2.5}{D_w^{\,2/3}} + \frac{1}{D_a^{\,2/3} \times Hprime} \right)^{-1}$$

Name	Description	Value
Kol	Overall mass transfer coefficient (cm/s)	Calculated above
beta	Proportionality constant (cm-s^-1/3)	216
Dw	Diffusion coefficient in water (cm^2/s)	Chemical-specific
Da	Diffusion coefficient in air (cm^2/s)	Chemical-specific
H*prime*	Dimensionless Henry's law constant (dimensionless)	Calculated in Equation E-3

This equation calculates the overall mass transfer coefficient. The above equation corresponds to Equation 17 in McKone (1987) and was modified to use the dimensionless Henry's law constant. McKone (1987) noted that the proportionality constant, beta, was a dimensionless value. Little (1992b) indicated that beta is not dimensionless. The correct units are noted above. The value for beta was derived using data for benzene and verified for chemicals of varying volatility (Coburn, 1996).

Equation E-6. Constituent mass emitted in the shower for a given time step

For Et > Emax,

$$\mathrm{Es} = \mathrm{Emax}$$

For Et $\leq$ Emax,

$$Es = Et$$

Where,

$$Et = Cin \times ShowerRate \times ts \times fem$$

$$\mathrm{Emax} = \left(y_{eq} - y_{s,\,t}\right) \times Vs \times 1000$$

Name	Description	Value
Es	Constituent mass emitted in the shower for a given time step (mg)	Calculated above
Emax	Maximum possible mass of constituent emitted from shower during time step (mg)	Calculated above
Et	Potential mass of constituent emitted from shower during time step (mg)	Calculated above
yeq	Gas-phase constituent concentration in equilibrium between water and air (mg/L)	H*prime* x Cin
ys, t	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated in Equation E-9 (As ys, t+ts for previous time step)
Vs	Volume of shower (m^3)	Provided in Table E-1
Cin	Liquid-phase constituent concentration in the incoming water (mg/L)	Provided in Table E-1
ShowerRate	Rate of flow from showerhead (L/min)	Provided in Table E-1
ts	Time step (min)	0.2
fem	Fraction of constituent emitted from a droplet (dimensionless)	Calculated in Equation E-7
H*prime*	Dimensionless Henry's law constant (dimensionless)	Calculated in Equation E-3
1000	Conversion factor (L/m^3)	Conversion factor

The above equations are used to determine the mass of constituent emitted for a given time step. The equilibrium concentration in air (y_eq) is calculated from Equation 1 in Little (1992a). If the mass emitted based on the mass transfer coefficient (Et) is greater than the amount emitted to reach equilibrium (Emax), the mass is set to the amount that results in the air concentration at equilibrium.

Equation E-7. Fraction of constituent emitted from a droplet

$$fem = \left(1 - Fsat\right) \times \left(1 - e^{-N}\right)$$

Name	Description	Value
fem	Fraction of constituent emitted from a droplet (dimensionless)	Calculated above
Fsat	Fraction of gas-phase saturation (dimensionless)	Calculated in Equation E-8
N	Dimensionless overall mass transfer coefficient (dimensionless)	Calculated in Equation E-4

This equation is used to calculate the fraction of a given chemical emitted from a droplet of water in the shower. The equation is based on Equation 5 in Little (1992a). The above equation is obtained by rearranging the equation in Little given that ys_max/m = Cin and Fsat = ys/ys_max = ys/(m × Cin).

Equation E-8. Fraction of gas-phase saturation in shower

$$Fsat = \frac{y_{s,\,t}}{y_{eq}}$$

Name	Description	Value
Fsat	Fraction of gas-phase saturation in shower (dimensionless)	Calculated above
yeq	Gas-phase constituent concentration in equilibrium between water and air (mg/L)	H*prime* x Cin
ys, t	Current gas-phase constituent concentration in air (mg/L)	Calculated in Equation E-9 (as ys, t+ts for previous time step)
H*prime*	Dimensionless Henry's law constant (dimensionless)	Calculated in Equation E-3
Cin	Constituent concentration in incoming water (mg/L)	Provided in Table E-1

This equation is used to calculate the fraction of gas phase saturation in shower for each time step. The equilibrium concentration in air (y_eq) is calculated from Equation 1 in Little (1992a).

Equation E-9. Gas-phase constituent concentration in the shower at end of time step

$$y_{s,\,t+ts} = y_{s,\,t} + \frac{\left[E_s - \left(Q_{sb} \times \left(y_{s,\,t} - y_{b,\,t}\right) \times ts\right)\right]}{V_s \times 1000}$$

Name	Description	Value
ys, t+ts	Gas-phase constituent concentration in the shower at end of time step (mg/L)	Calculated above
ys, t	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated in Equation E-10 (as yb, t+ts for previous time step)
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
Es	Mass emitted in the shower for a given time step (mg)	Calculated in Equation E-6
Qsb	Volumetric exchange rate between the shower and the bathroom (L/min)	Provided in Table E-1
Vs	Volume of shower (m^3)	Provided in Table E-1
ts	Time step (min)	0.2
1000	Conversion factor (L/m^3)	Conversion factor

This equation is used to calculate the gas-phase constituent concentration in the shower at end of time step. The equation is derived from Equation 9 in Little (1992a). Es is set to 0 when the shower is turned off (i.e., at the end of showering) to estimate the reduction in shower stall air concentrations after emissions cease.

Equation E-10. Gas-phase constituent concentration in the bathroom at end of time step

$$y_{b,\,t+ts} = y_{b,\,t} + \frac{\left[\left(Q_{sb} \times \left(y_{s,\,t+ts} - y_{b,\,t}\right) - Q_{bh} \times \left(y_{b,\,t} - y_{h,\,t}\right)\right)\right]}{V_b \times 1000} \times ts$$

Name	**Description**	**Value**
yb, t+ts	Gas-phase constituent concentration in the bathroom at end of time step (mg/L)	Calculated above
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
ys, t+ts	Gas-phase constituent concentration in the shower at the end of time step (mg/L)	Calculated in Equation E-9
yh, t	Gas-phase constituent concentration in the house at the beginning of time step (mg/L)	Assumed deminimus, zero
Qsb	Volumetric exchange rate between the shower and the bathroom (L/min)	Provided in Table E-1
Qbh	Volumetric exchange rate between the bathroom and the house (L/min)	Provided in Table E-1
Vb	Volume of bathroom (m^3)	Provided in Table E-1
ts	Time step (min)	0.2
1000	Conversion factor (L/m^3)	Conversion factor

This equation is used to calculate the gas-phase constituent concentration in the bathroom at end of time step. The equation is derived from Equation 10 in Little (1992a).

Equation E-11. Average daily concentration in indoor air

$$Cair\_indoor = \frac{\left(Cair\_shower \times ShowerResTime\right) + \left(Cair\_bathroom \times T\_bathroom\right)}{1440}$$

$$Cair\_shower = \frac{\sum \left[\left(ys_{,\,t+ts} + ys_{,\,t}\right)/2\right] \times 1000}{ns}$$

$$Cair\_bathroom = \frac{\sum \left[\left(yb_{,\,t+ts} + yb_{,t}\right)/2\right] \times 1000}{nb}$$

Name	Description	Value
Cair_indoor	Average daily concentration in indoor air (mg/m^3)	Calculated above
Cair_shower	Average concentration in shower (mg/m^3)	Calculated above
Cair_bathroom	Average concentration in bathroom (mg/m^3)	Calculated above
ShowerResTime	Total time spent in shower stall (min)	Calculated in Equation E-2
T_bathroom	Time spent in bathroom, not in shower (min)	Provided in Table E-1
ys, t	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated in Equation E-9 (as ys, t+ts for previous time step)
ys, t+ts	Gas-phase constituent concentration in the shower at the end of time step (mg/L)	Calculated in Equation E-9
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated in Equation E-10 (as yb, t+ts for previous time step)
yb, t+ts	Gas-phase constituent concentration in the bathroom at the end of time step (mg/L)	Calculated in Equation E-10
ns	Number of time steps corresponding to time spent in the shower (dimensionless)	Summed in model code
nb	Number of time steps corresponding to time spent in the bathroom (dimensionless)	Summed in model code
1440	Minutes per day (min)	Adjustment factor
1000	Conversion factor (L/m^3)	Conversion factor

The above equations are used to calculate the time-weighted average daily indoor air concentration to which a receptor is exposed. The equation assumes that receptors are only exposed to constituents in the shower and bathroom.

E-1.3 References for Section E-1

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E-2 Constituent-specific Chemical and Physical Properties for the Shower Model

To calculate inhalation HBNs, the shower model requires input of several chemical-specific properties, including solubility *(Sol)*, Henry's law constant *(HLC)*, and diffusion coefficients in air (D_a) and water (D_w). This attachment describes the data sources and methodologies used to collect and develop these properties. Table E.2 lists by constituent the chemical-specific properties used to calculate inhalation HBNs, along with the data source for each value.

E-2.1 Data Collection Procedure

To select data values available from multiple sources, we created a hierarchy of references based on the reliability and availability of data in such sources. Our first choice for data collection and calculations was EPA reports and software. When we could not find data or equations from EPA publications, we consulted highly recognized sources, including chemical information databases on the Internet. These on-line sources are compilations of data that provide the primary references for data values. The specific hierarchy varied among properties as described in subsequent sections.

For dioxins, the preferred data source in all cases was the *Exposure and Human Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds, Part 1, Vol. 3* (*Dioxin Reassessment*) (U.S. EPA, 2000). We used the *Mercury Study Report to Congress* (U.S. EPA, 1997a) as the preferred source for mercury properties. If values were unavailable from these sources, we followed the same reference hierarchy that was used for other constituents.

All data entry for chemical and physical properties was checked by comparing each entry against the original online or hardcopy reference. All property calculation programs were checked using hand calculations to ensure that they were functioning correctly.

E-2.2 Solubility (Sol)

For solubility *(Sol)* values, we looked for data by searching the following sources in the following order:

1. Superfund Chemical Data Matrix (SCDM) (U.S. EPA, 1997b);
2. CHEMFATE Chemical Search (SRC, 1999);
3. Hazardous Substances Data Bank (HSDB) (U.S. NLM, 2001);
4. ChemFinder (CambridgeSoft Corporation, 2001).

For mercury, we obtained a solubility for elemental mercury from *The Merck Index*: *An Encyclopedia of Chemicals, Drugs, and Biologicals* (Budavari, 1996).

E-2.3 Henry's Law Constant (HLC)

Collection of Henry's law constant *(HLC)* data proceeded by searching sources in the following order:

1. SCDM;
2. CHEMFATE;
3. HSDB.

When we could not find data from these sources, we calculated HLC using equation 15-8 from Lyman, Reehl, and Rosenblatt (1990):

$$HLC = \frac{P_{vp}}{Sol}$$

where

HLC = Henry's law constant (atm-m^3/mole)
P_{vp} = vapor pressure (atm)
Sol = solubility (mol/m^3).

E-2.4 Diffusion Coefficient in Water (D_w)

For all chemicals, we calculated the diffusion coefficient in water (D_w) by hand because few empirical data are available. The preferred calculation was equation 17-6 from the WATER9 model (U.S. EPA, 2001):

$$D_w = 0.0001518\left(\frac{T+273.16}{298.16}\right)\left(\frac{MW}{\rho}\right)^{-0.6}$$

where

D_w = diffusion coefficient in water (cm^2/s)
T = temperature (degrees C)
MW = molecular weight (g/g-mol)
ρ = density (g/cc).

When we did not know chemical density, we used equation 3.16 from *Process Coefficients and Models for Simulating Toxic Organics and Heavy Metals in Surface Waters (Process Coefficients)* (U.S. EPA, 1987), which only requires molecular weight:

$$Dw = 0.00022 \times MW^{-2/3}$$

where

D_w = diffusion coefficient in water (cm^2/s)
MW = molecular weight (g/mol).

E-2.5 Diffusion Coefficient in Air (D_a)

All diffusion coefficients in air (D_a) were calculated values because few empirical data are available. Similar to D_w, we first consulted WATER9 and then used U.S. EPA (1987). Equation 17-5 in WATER9 calculates diffusivity in air as follows:

$$D_a = \frac{0.0029(T + 273.16)^{1.5}\sqrt{0.034 + \frac{1}{MW}}\left(1 - 0.000015MW^2\right)}{\left[\left(\frac{MW}{2.5\rho}\right)^{0.333} + 1.8\right]^2}$$

where

D_a = diffusion coefficient in air (cm^2/s)
T = temperature (degrees C)
MW = molecular weight (g/g-mol)
ρ = density (g/cc).

When density was not available, we used equation 3.17 from Process Coefficients (U.S. EPA, 1987):

$$Da = 1.9 \times MW^{-2/3}$$

where

D_a = diffusion coefficient in air (cm^2/s)
MW = molecular weight (g/mol).

For dioxins and furans, we used an equation from the Dioxin Reassessment (U.S. EPA, 2000) to estimate diffusion coefficients from diphenyl's diffusivity:

$$\frac{D_a}{D_b} = \left(\frac{MW_b}{MW_a}\right)^{0.5}$$

where

D_a = diffusion coefficient of constituent in air (cm^2/s)
D_b = diffusion coefficient of diphenyl at 25 degrees C (0.068 cm^2/s)
MW_a = molecular weight of constituent (g/mole)
MW_b = molecular weight of diphenyl (154 g/mole).

Table E-2. Constituent-specific Chemical and Physical Properties

Constituent	CASRN	D_a (cm^2/s) (a)	D_w (cm^2/s) (a)	HLC (atm-m^3/mol) (c)	Sol (mg/L) (c)
Acetaldehyde (ethanal)	75-07-0	0.128	0	7.89e-05	1.00e+06
Acetone (2-propanone)	67-64-1	1.06E-01	1.15E-05	3.88e-05	1.00e+06
Acetonitrile (methyl cyanide)	75-05-8	1.34E-01	1.41E-05	3.46e-05	1.00e+06
Acrolein	107-02-8	1.12E-01	1.22E-05	1.22e-04	2.13e+05
Acrylamide	79-06-1	1.07E-01	1.26E-05	1.00e-09	6.40e+05
Acrylic acid (propenoic acid)	79-10-7	1.03E-01	1.20E-05	1.17e-07	1.00e+06
Acrylonitrile	107-13-1	1.14E-01	1.23E-05	1.03e-04	7.40e+04
Aldrin	309-00-2	2.28E-02	5.84E-06	1.70e-04	1.80e-01
Aniline (benzeneamine)	62-53-3	8.30E-02	1.01E-05	1.90e-06	3.60e+04
Benz(a)anthracene	56-55-3	5.09E-02[b]	5.89E-06[b]	3.35e-06	9.40e-03
Benzene	71-43-2	8.95E-02	1.03E-05	5.55e-03	1.75e+03
Benzidine	92-87-5	3.55E-02	7.59E-06	3.88e-11	5.00e+02
Benzo(a)pyrene	50-32-8	2.55E-02	6.58E-06	1.13e-06	1.62e-03
Benzo(b)fluoranthene	205-99-2	4.76E-02[b]	5.51E-06[b]	1.11e-04	1.50e-03
Benzyl chloride	100-44-7	6.34E-02	8.81E-06	4.15e-04	5.25e+02
Bis(2-ethylhexyl)phthalate	117-81-7	1.73E-02	4.18E-06	1.02e-07	3.40e-01
Bis(2-chloroethyl)ether	111-44-4	5.67E-02	8.71E-06	1.80e-05	1.72e+04
Bis(2-chloroisopropyl)ether	39638-32-9	4.01E-02	7.40E-06	1.34e-04[e]	1.31e+03
Bromodichloromethane	75-27-4	5.63E-02	1.07E-05	1.60e-03	6.74e+03
Bromomethane (methyl bromide)	74-83-9	1.00E-01	1.35E-05	6.24e-03	1.52e+04
Butadiene, 1,3-	106-99-0	1.00E-01	1.03E-05	7.36e-02	7.35e+02
Carbon tetrachloride	56-23-5	5.71E-02	9.78E-06	3.04e-02	7.93e+02
Carbon disulfide	75-15-0	1.06E-01	1.30E-05	3.03e-02	1.19e+03
Chlordane	57-74-9	2.15E-02	0	4.86e-05	5.60e-02
Chloro-1,3-butadiene, 2- (Chloroprene)	126-99-8	8.41E-02	1.00E-05	1.19e-02[f]	1.74e+03
Chlorobenzene	108-90-7	7.21E-02	9.48E-06	3.70e-03	4.72e+02
Chlorobenzilate	510-15-6	2.18E-02	5.48E-06	7.24e-08[f]	1.11e+01
Chlorodibromomethane	124-48-1	3.66E-02	1.06E-05	7.83e-04	2.60e+03
Chloroethane (ethyl chloride)	75-00-3	1.04E-01	1.16E-05	8.82e-03	5.68e+03
Chloroform	67-66-3	7.70E-02	1.09E-05	3.67e-03	7.92e+03

Table E-2. Constituent-specific Chemical and Physical Properties (continued)

Constituent	CASRN	D_a (cm^2/s) (a)	D_w (cm^2/s) (a)	HLC (atm-m^3/mol) (c)	Sol (mg/L) (c)
Chloromethane (methyl chloride)	74-87-3	0.124	1.36E-05	8.82e-03	5.33e+03
Chlorophenol, 2-	95-57-8	0.0661	0	3.91e-04	2.20e+04
Chloropropene, 3- (allyl chloride)	107-05-1	9.36E-02	1.08E-05	1.10e-02	3.37e+03
Chrysene	218-01-9	2.61E-02	6.75E-06	9.46e-05	1.60e-03
Cresol, o-	95-48-7	7.59E-02	9.86E-06	1.20e-06	2.60e+04
Cresol, —	108-39-4	0.0729	0	8.65e-07	2.27e+04
Cresol, p-	106-44-5	7.24E-02	9.24E-06	7.92e-07	2.15e+04
Cresols (total)	1319-77-3	7.37E-02	9.48E-06	9.52e-07	2.34e+04
Cumene	98-82-8	6.02E-02	7.85E-06	1.16e+00	6.13e+01
Cyclohexanol	108-93-0	7.59E-02	9.35E-06	1.02e-04[f]	4.30e+04[f]
DDT, p,p'-	50-29-3	1.83E-02	4.44E-06	8.10e-06	2.50e-02
Dibenz(a,h)anthracene	53-70-3	0.0236	6.02E-06	1.47e-08	2.49e-03
Dibromo-3-chloropropane, 1,2-	96-12-8	0.0321	8.90E-06	1.47e-04	1.23e+03
Dichlorobenzene, 1,2-	95-50-1	0.0562	8.92E-06	1.90e-03	1.56e+02
Dichlorobenzene, 1,4-	106-46-7	0.055	8.68E-06	2.40e-03	7.38e+01
Dichlorobenzidine, 3,3'-	91-94-1	4.75E-02[b]	5.50E-06[b]	4.00e-09	3.11e+00
Dichlorodifluoromethane (Freon 12)	75-71-8	7.60E-02	1.08E-05	3.43e-01	2.80e+02
Dichloroethane, 1,1-	75-34-3	8.36E-02	1.06E-05	5.62e-03	5.06e+03
Dichloroethane, 1,2-	107-06-2	8.54E-02	1.09E-05	9.79e-04	8.52e+03
Dichloroethylene, 1,1-	75-35-4	8.63E-02	1.10E-05	2.61e-02	2.25e+03
Dichloropropane, 1,2-	78-87-5	7.33E-02	9.73E-06	2.80e-03	2.80e+03
Dichloropropene, trans-1,3-	10061-02-6	7.63E-02	1.01E-05	1.80e-03[i]	2.72e+03
Dichloropropene, 1,3- (isomer mixture)	542-75-6	7.63E-02	1.01E-05	1.77e-02	2.80e+03
Dichloropropene, cis-1,3-	10061-01-5	7.65E-02	1.02E-05	2.40e-03[i]	2.72e+03
Dieldrin	60-57-1	2.33E-02	6.01E-06	1.51e-05	1.95e-01
Dimethyl formamide, N,N- (DMF)	68-12-2	9.72E-02	1.12E-05	7.39e-08[i]	1.00e+06[f]
Dimethylbenz(a)anthracene, 7,12-	57-97-6	4.71E-02[b]	5.45E-06[b]	3.11e-08	2.50e-02
Dinitrotoluene, 2,4-	121-14-2	3.75E-02	7.90E-06	9.26e-08	2.70e+02
Dioxane, 1,4-	123-91-1	8.74E-02	1.05E-05	4.80e-06	1.00e+06
Diphenylhydrazine, 1,2-	122-66-7	0.0343	7.25E-06	1.53e-06	6.80e+01
Epichlorohydrin	106-89-8	0.0888	1.11E-05	3.04e-05	6.59e+04

Table E-2. Constituent-specific Chemical and Physical Properties (continued)

Constituent	CASRN	D_a (cm^2/s) (a)	D_w (cm^2/s) (a)	HLC (atm-m^3/mol) (c)	Sol (mg/L) (c)
Epoxybutane, 1,2-	106-88-7	9.32E-02	1.05E-05	1.80e-04[f]	9.50e+04[f]
Ethoxyethanol acetate, 2-	111-15-9	0.057	0	1.80e-06[i]	2.29e+05[i]
Ethoxyethanol , 2-	110-80-5	8.19E-02	9.76E-06	1.23e-07	1.00e+06
Ethylbenzene	100-41-4	6.86E-02	8.48E-06	7.88e-03	1.69e+02
Ethylene dibromide (1,2-dibromoethane)	106-93-4	4.31E-02	1.05E-05	7.43e-04	4.18e+03
Ethylene glycol	107-21-1	1.17E-01	1.36E-05	6.00e-08	1.00e+06
Ethylene thiourea	96-45-7	8.69E-02	1.01E-05	3.08e-10	6.20e+04
Ethylene oxide	75-21-8	1.34E-01	1.46E-05	1.48e-04	1.00e+06[g]
Formaldehyde	50-00-0	1.67E-01	1.74E-05	3.36e-07	5.50e+05
Furfural	98-01-1	8.53E-02	1.07E-05	4.00e-06	1.10e+05
HCH, gamma- (Lindane)	58-89-9	2.74E-02	7.30E-06	1.40e-05	6.80e+00
HCH, beta-	319-85-7	0.0277	7.40E-06	7.43e-07	2.40e-01
HCH, alpha-	319-84-6	2.75E-02	7.35E-06	1.06e-05	2.00e+00
Heptachlor epoxide	1024-57-3	2.19E-02	5.58E-06	9.50e-06	2.00e-01
Heptachlor	76-44-8	2.23E-02	5.70E-06	1.10e-03	1.80e-01
Hexachloro-1,3-butadiene	87-68-3	2.67E-02	7.03E-06	8.15e-03	3.23e+00
Hexachlorobenzene	118-74-1	2.90E-02	7.85E-06	1.32e-03	5.00e-03
Hexachlorocyclopentadiene	77-47-4	2.72E-02	7.22E-06	2.70e-02	1.80e+00
Hexachlorodibenzo-p-dioxins (HxCDDs)	34465-46-8	4.27E-02[j]	4.12E-06[b]	1.10e-05[d]	4.40e-06[d]
Hexachlorodibenzofurans (HxCDFs)	55684-94-1	4.36E-02[j]	4.23E-06[b]	1.10e-05[d]	1.30e-05[d]
Hexachloroethane	67-72-1	3.21E-02	8.89E-06	3.89e-03	5.00e+01
Hexane	110-54-3	7.28E-02	8.12E-06	1.43e-02	1.24e+01
Indeno(1,2,3-cd)pyrene	193-39-5	4.48E-02	5.19E-06	1.60e-06	2.20e-05
Isophorone	78-59-1	5.25E-02	7.53E-06	6.64e-06	1.20e+04
Mercury	7439-97-6	7.15E-02	3.01E-05	7.10e-03[k]	5.62e-02[h]
Methacrylonitrile	126-98-7	9.64E-02	1.06E-05	2.47e-04	2.54e+04
Methanol	67-56-1	1.58E-01	1.65E-05	4.55e-06	1.00e+06
Methoxyethanol acetate, 2-	110-49-6	6.59E-02	8.71E-06	3.11e-07[e]	1.00e+06[i]
Methoxyethanol, 2-	109-86-4	0.0952	1.10E-05	8.10e-08[f]	1.00e+06[g]
Methyl methacrylate	80-62-6	7.53E-02	9.25E-06	3.37e-04	1.50e+04

Table E-2. Constituent-specific Chemical and Physical Properties (continued)

Constituent	CASRN	D_a (cm^2/s) (a)	D_w (cm^2/s) (a)	HLC (atm-m^3/mol) (c)	Sol (mg/L) (c)
Methyl tert-butyl ether (MTBE)	1634-04-4	0.0755	0	5.87e-04[f]	5.13e+04[f]
Methyl isobutyl ketone	108-10-1	0.0698	0	1.38e-04	1.90e+04
Methyl ethyl ketone	78-93-3	0.0917	0	5.59e-05	2.23e+05
Methylcholanthrene, 3-	56-49-5	2.41E-02	6.14E-06	9.40e-07	3.23e-03
Methylene chloride (dichloromethane)	75-09-2	9.99E-02	1.25E-05	2.19e-03	1.30e+04
N-Nitrosomethylethylamine	10595-95-6	8.41E-02	9.99E-06	1.40e-06[i]	1.97e+04
N-Nitrosodimethylamine	62-75-9	9.88E-02	1.15E-05	1.20e-06	1.00e+06
N-Nitrosopiperidine	100-75-4	6.99E-02	9.18E-06	2.80e-07	7.65e+04
N-Nitrosodiphenylamine	86-30-6	2.84E-02	7.19E-06	5.00e-06	3.51e+01
N-Nitrosodiethylamine	55-18-5	7.38E-02	9.13E-06	3.63e-06	9.30e+04
N-Nitroso-di-n-butylamine	924-16-3	4.22E-02	6.83E-06	3.16e-04	1.27e+03
N-Nitrosopyrrolidine	930-55-2	8.00E-02	1.01E-05	1.20e-08	1.00e+06
N-Nitroso-di-n-propylamine	621-64-7	5.64E-02	7.76E-06	2.25e-06	9.89e+03
Naphthalene	91-20-3	6.05E-02	8.38E-06	4.83e-04	3.10e+01
Nitrobenzene	98-95-3	6.81E-02	9.45E-06	2.40e-05	2.09e+03
Nitropropane, 2-	79-46-9	8.47E-02	1.02E-05	1.23e-04	1.70e+04
Pentachlorodibenzo-p-dioxins (PeCDDs)	36088-22-9	0.0447[j]	4.38E-06[b]	2.60e-06[d]	1.18e-04[d]
Pentachlorodibenzofurans (PeCDFs)	30402-15-4	4.57E-02[j]	4.51E-06[b]	5.00e-06[d]	2.40e-04[d]
Pentachlorophenol	87-86-5	2.95E-02	8.01E-06	2.44e-08	1.95e+03
Phenol	108-95-2	8.34E-02	1.03E-05	3.97e-07	8.28e+04
Phthalic anhydride	85-44-9	5.95E-02	9.75E-06	1.63e-08	6.20e+03
Polychlorinated biphenyls (Aroclors)	1336-36-3	2.33E-02	5.98E-06	2.60e-03	7.00e-02
Propylene oxide (1,2-epoxypropane)	75-56-9	1.10E-01	1.21E-05	1.23e-04[f]	4.05e+05[f]
Pyridine	110-86-1	9.31E-02	1.09E-05	8.88e-06	1.00e+06
Styrene	100-42-5	7.13E-02	8.81E-06	2.75e-03	3.10e+02
Tetrachlorodibenzo-p-dioxin, 2,3,7,8- (2,3,7,8-TCDD)	1746-01-6	4.70E-02[j]	4.68E-06[b]	3.29e-05[d]	1.93e-05[d]
Tetrachlorodibenzofurans (TCDFs)*	55722-27-5	4.82E-02[j]	4.84E-06[b]	1.40e-05[d]	4.20e-04[d]
Tetrachloroethane, 1,1,2,2-	79-34-5	4.89E-02	9.29E-06	3.45e-04	2.97e+03
Tetrachloroethane, 1,1,1,2-	630-20-6	4.82E-02	9.10E-06	2.42e-03	1.10e+03
Tetrachloroethylene	127-18-4	5.05E-02	9.45E-06	1.84e-02	2.00e+02

Table E-2. Constituent-specific Chemical and Physical Properties (continued)

Constituent	CASRN	D_a (cm^2/s) (a)	D_w (cm^2/s) (a)	HLC (atm-m^3/mol) (c)	Sol (mg/L) (c)
Toluene	108-88-3	0.078	0	6.64e-03	5.26e+02
Toluenediamine 2,4-	95-80-7	7.72E-02[b]	8.94E-06[b]	7.92e-10	3.37e+04
Toluidine, o-	95-53-4	0.0724	0	2.72e-06	1.66e+04
Toxaphene (chlorinated camphenes)	8001-35-2	0.0216	0	6.00e-06	7.40e-01
Tribromomethane (bromoform)	75-25-2	3.58E-02	1.04E-05	5.35e-04	3.10e+03
Trichloro-1,2,2-trifluoro-ethane, 1,1,2-	76-13-1	3.76E-02	8.59E-06	4.81e-01	1.70e+02
Trichlorobenzene, 1,2,4-	120-82-1	3.96E-02	8.40E-06	1.42e-03	3.46e+01
Trichloroethane, 1,1,2-	79-00-5	6.69E-02	1.00E-05	9.13e-04	4.42e+03
Trichloroethane, 1,1,1-	71-55-6	6.48E-02	9.60E-06	1.72e-02	1.33e+03
Trichloroethylene (TCE)	79-01-6	6.87E-02	1.02E-05	1.03e-02	1.10e+03
Trichlorofluoromethane (Freon 11)	75-69-4	6.55E-02	1.01E-05	9.70e-02	1.10e+03
Trichlorophenol, 2,4,6-	88-06-2	3.14E-02	8.09E-06	7.79e-06	8.00e+02
Trichloropropane, 1,2,3-	96-18-4	5.75E-02	9.24E-06	4.09e-04	1.75e+03
Triethylamine	121-44-8	6.63E-02	7.84E-06	1.38e-04[f]	5.50e+04[f]
Vinyl acetate	108-05-4	8.51E-02	1.00E-05	5.11e-04	2.00e+04
Vinyl chloride	75-01-4	1.07E-01	1.20E-05	2.70e-02	2.76e+03
Xylene, p-	106-42-3	6.84E-02	8.45E-06	7.66e-03	1.85e+02
Xylene, o-	95-47-6	6.91E-02	8.56E-06	5.19e-03	1.78e+02
Xylene, m-	108-38-3	6.85E-02	8.47E-06	7.34e-03	1.61e+02
Xylenes (total)	1330-20-7	0.0687	0	6.73e-03	1.75e+02

D_a = air diffusivity; D_w = water diffusivity; HLC = Henry's law constant; Sol = aqueous solubility
CASRN = Chemical Abstract Service Registry Number
* Values used for 2,3,7,8-tetrachlorodibenzofuran (CAS #51207-31-9).
Data Sources:
[a] Calculated based on WATER9 (U.S. EPA, 2001).
[b] Calculated based on U.S. EPA, 1987.
[c] SCDM (U.S. EPA, 1997b).
[d] U.S. EPA, 2000.
[e] Calculated based on Lyman, Reehl, and Rosenblatt, 1990.
[f] CHEMFATE (SRC, 1999).
[g] ChemFinder.com (CambridgeSoft Corporation, 2001).
[h] The Merck Index (Budavari, 1996).
[i] HSDB (U.S. NLM, 2001).
[j] Calculated based on U.S. EPA, 2000.
[k] U.S. EPA, 1997a.

E-2.6 References for Section E-2

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E-3 Human Health Benchmarks used in the IWEM Tool

Human health benchmarks for chronic oral and inhalation exposures are an important component of the IWEM 1 tool. The EPA uses reference doses (RfDs) and reference concentrations (RfCs) to evaluate noncancer risk from oral and inhalation exposures, respectively. Oral cancer slope factors (CSFs), inhalation unit risk factors (URFs), and inhalation CSFs are used to evaluate risk for carcinogens.

This section provides the toxicity benchmarks we used to develop the HBNs that we will use in developing Reference Ground-Water Concentrations for IWEM. Section E-3.1 describes the data sources and general hierarchy used to collect these benchmarks. Section E-3.2 provides the benchmarks along with discussions of individual human health benchmarks extracted from a variety of sources.

E-3.1 Methodology and Data Sources

Several sources of health benchmarks are available. Human health benchmarks were obtained from these sources in the following order of preference:

- Integrated Risk Information System (IRIS)
- Superfund Technical Support Center Provisional Benchmarks
- Health Effects Assessment Summary Tables (HEAST)
- Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs)
- California Environmental Protection Agency (CalEPA) chronic inhalation reference exposure levels (RELs) and cancer potency factors.
- EPA health assessment documents
- Various other EPA health benchmark sources.

For dioxins and dibenzofurans, World Health Organization (WHO) toxicity equivalency factors (TEFs) from Van den Berg et al. (1998) were applied to the oral and inhalation CSF for 2,3,7,8-TCDD to obtain CSFs for all other dioxins and furans (see Section E-3.2.4).

E-3.1.1 Integrated Risk Information System (IRIS)

Benchmarks in IRIS are prepared and maintained by EPA, and values from IRIS were used to develop HBNs for the IWEM tool whenever IRIS benchmarks were available. IRIS is EPA’s electronic database containing information on human health effects (U.S. EPA, 2001a). Each chemical file contains descriptive and quantitative information on potential health effects. Health benchmarks for chronic noncarcinogenic health effects include RfDs and RfCs. Cancer classification, oral CSFs, and inhalation

URFs are included for carcinogenic effects. IRIS is the official repository of Agency-wide consensus of human health risk information.

Inhalation CSFs are not available from IRIS, so they were calculated from inhalation URFs (which are available from IRIS) using the following equation:

$$\text{inh CSF} = \text{inh URF} \times 70 \text{ kg} \div 20 \text{ m}^3/\text{d} \times 1000 \ \mu\text{g/mg}$$

In this equation, 70 kg represents average body weight; 20 m^3/d represents average inhalation rate; and 1000 µg/mg is a units conversion factor (U.S. EPA, 1997). These standard estimates of body weight and inhalation rate are used by EPA in the calculation of the URF, and, therefore, the values were used to calculate inhalation CSFs.

E-3.1.2 Superfund Provisional Benchmarks

The Superfund Technical Support Center (EPA's National Center for Environmental Assessment [NCEA]) derives provisional RfCs, RfDs, and CSFs for certain chemicals. These provisional health benchmarks can be found in Risk Assessment Issue Papers. Some of the provisional values have been externally peer reviewed, and some (e.g., trichloroethylene, tetrachloroethylene) come from previously published EPA Health Assessment Documents. These provisional values have not undergone EPA's formal review process for finalizing benchmarks and do not represent Agency-wide consensus information. Specific provisional values used in the IWEM tool are described in Section E-3.2.5.

E-3.1.3 Health Effects Summary Tables (HEAST)

HEAST is a listing of provisional noncarcinogenic and carcinogenic health toxicity values (RfDs, RfCs, URFs, and CSFs) derived by EPA (U.S. EPA, 1997). Although the health toxicity values in HEAST have undergone review and have the concurrence of individual EPA program offices, either they have not been reviewed as extensively as those in IRIS or their data set is not complete enough to be listed in IRIS. HEAST benchmarks have not been updated in several years and do not represent Agency-wide consensus information.

E-3.1.4 ATSDR Minimal Risk Levels

The ATSDR MRLs are substance-specific health guidance levels for noncarcinogenic endpoints (ATSDR, 2001). An MRL is an estimate of the daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse noncancer health effects over a specified duration of exposure. MRLs are based on noncancer health effects only and are not based on a consideration of cancer effects.

MRLs are derived for acute, intermediate, and chronic exposure durations for oral and inhalation routes of exposure. Inhalation and oral MRLs are derived in a manner similar to EPA's RfCs and RfDs, respectively (i.e., ATSDR uses the no-observed-adverse-effect-level/uncertainty factor (NOAEL/UF) approach); however, MRLs are intended to serve as screening levels and are exposure duration-specific. Also, ATSDR uses EPA's 1994 inhalation dosimetry methodology in the derivation of inhalation MRLs. A chronic inhalation MRL for mixed xylenes was used as a surrogate for each of the xylene isomers.

E-3.1.5 CalEPA Cancer Potency Factors and Reference Exposure Levels

CalEPA has developed cancer potency factors for chemicals regulated under California's Hot Spots Air Toxics Program (CalEPA, 1999a). The cancer potency factors are analogous to EPA's oral and inhalation CSFs. CalEPA has also developed chronic inhalation RELs, analogous to EPA's RfC, for 120 substances (CalEPA, 1999b, 2000). CalEPA used EPA's 1994 inhalation dosimetry methodology in the derivation of inhalation RELs. The cancer potency factors and inhalation RELs have undergone internal peer review by various California agencies and have been the subject of public comment. A chronic inhalation REL for mixed cresols was used as a surrogate for each of the cresol isomers.

E-3.1.6 Other EPA Health Benchmarks

EPA has also derived health benchmark values in other risk assessment documents, such as Health Assessment Documents (HADs), Health Effect Assessments (HEAs), Health and Environmental Effects Profiles (HEEPs), Health and Environmental Effects Documents (HEEDs), Drinking Water Criteria Documents, and Ambient Water Quality Criteria Documents. Evaluations of potential carcinogenicity of chemicals in support of reportable quantity adjustments were published by EPA's Carcinogen Assessment Group (CAG) and may include cancer potency factor estimates. Health toxicity values identified in these EPA documents are usually dated and are not recognized as Agency-wide consensus information or verified benchmarks, however, and as a result they are used in the hierarchy only when values are not available from IRIS, HEAST, Superfund provisional values, ATSDR, or CalEPA. Section E-3.2.6 describes the specific values from these alternative EPA sources that were used in the IWEM tool.

E-3.2 Human Health Benchmark Values

The chronic human health benchmarks used to calculate the HBNs in the IWEM tool are summarized in Table E-3, which provides the Chemical Abstract Service Registry Number (CASRN), constituent name, RfD (mg/kg-d), RfC (mg/m^3), oral CSF (mg/kg-d^{-1}), inhalation URF [(µg/m^3)$^{-1}$], inhalation CSF (mg/kg-d^{-1}), and reference for each benchmark. A key to the references cited and abbreviations used is provided at the end of the table.

For a majority of the IWEM constituents, human health benchmarks were available from IRIS (U.S. EPA, 2001a), Superfund Provisional Benchmarks, or HEAST (U.S. EPA, 1997). Benchmarks also were obtained from ATSDR (2001) or CalEPA (1999a, 1999b, 2000). This section describes benchmarks obtained from other sources, along with the Superfund Provisional values and special uses (e.g., benzene, vinyl chloride) of IRIS benchmarks.

Table E-3. Human Health Benchmark Values

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Acenaphthene	83-32-9	6.0E-02	I								
Acetaldehyde (ethanal)	75-07-0					9.0E-03	I	2.2E-06	I	7.7E-03	calc
Acetone (2-propanone)	67-64-1	1.0E-01	I			3.1E+01	A				
Acetonitrile (methyl cyanide)	75-05-8					6.0E-02	I				
Acetophenone	98-86-2	1.0E-01	I								
Acrolein	107-02-8	2.0E-02	H			2.0E-05	I				
Acrylamide	79-06-1	2.0E-04	I	4.5E+0	I			1.3E-03	I	4.6E+00	calc
Acrylic acid (propenoic acid)	79-10-7	5.0E-01	I			1.0E-03	I				
Acrylonitrile	107-13-1	1.0E-03	H	5.4E-1	I	2.0E-03	I	6.8E-05	I	2.4E-01	calc
Aldrin	309-00-2	3.0E-05	I	1.7E+01	I			4.9E-03	I	1.7E+01	calc
Allyl alcohol	107-18-6	5.0E-03	I								
Aniline (benzeneamine)	62-53-3			5.7E-3	I	1.0E-03	I	1.6E-06	C99a	5.6E-03	calc
Anthracene	120-12-7	3.0E-01	I								
Antimony	7440-36-0	4.0E-04	I								
Arsenic	7440-38-2	3.0E-04	I	1.5E+00	I						
Barium	7440-39-3	7.0E-02	I								
Benz{a}anthracene	56-55-3			1.2E+00	C99a			1.1E-04	C99a	3.9E-01	calc
Benzene	71-43-2			5.5E-02	I	6.0E-02	C00	7.8E-06	I	2.7E-02	calc
Benzidine	92-87-5	3.0E-03	I	2.3E+02	I			6.7E-02	I	2.3E+02	I
Benzo{a}pyrene	50-32-8			7.3E+00	I			1.1E-03	C99a	3.9E+00	calc
Benzo{b}fluoranthene	205-99-2			1.2E+00	C99a			1.1E-04	C99a	3.9E-01	calc
Benzyl chloride	100-44-7			1.7E-01	I			4.9E-05	C99a	1.7E-01	calc
Benzyl alcohol	100-51-6	3.0E-01	H								
Beryllium	7440-41-7	2.0E-03	I								
Bis(2-chloroethyl)ether	111-44-4			1.1E+00	I			3.3E-04	I	1.2E+00	calc

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Bis(2-chloroisopropyl)ether	39638-32-9	4.0E-02	I	7.0E-02	H			1.0E-05	H	3.5E-02	calc
Bis(2-ethylhexyl)phthalate	117-81-7	2.0E-02	I	1.4E-02	I	1.0E-02	C99b	2.4E-06	C99a	8.4E-03	calc
Bromodichloromethane	75-27-4	2.0E-02	I	6.2E-02	I			1.8E-05	AC	6.2E-02	AC
Bromomethane (methyl bromide)	74-83-9	1.4E-03	I			5.0E-03	I				
Butadiene, 1,3-	106-99-0					2.0E-02	C00	2.8E-04	I	9.8E-01	calc
Butanol	71-36-3	1.0E-01	I								
Butyl benzyl phthalate	85-68-7	2.0E-01	I								
Butyl-4,6-dinitrophenol,2-sec- (Dinoseb)	88-85-7	1.0E-03	I								
Cadmium	7440-43-9	5.0E-04	I								
Carbon tetrachloride	56-23-5	7.0E-04	I	1.3E-01	I	7.0E-03	SF	1.5E-05	I	5.3E-02	calc
Carbon disulfide	75-15-0	1.0E-01	I			7.0E-01	I				
Chlordane	57-74-9	5.0E-04	I	3.5E-01	I	7.0E-04	I	1.0E-04	I	3.5E-01	calc
Chloro-1,3-butadiene, 2- (Chloroprene)	126-99-8	2.0E-02	H			7.0E-03	H				
Chloroaniline, p-	106-47-8	4.0E-03	I								
Chlorobenzene	108-90-7	2.0E-02	I			6.0E-02	SF				
Chlorobenzilate	510-15-6	2.0E-02	I	2.7E-01	H			7.8E-05	H	2.7E-01	calc
Chlorodibromomethane	124-48-1	2.0E-02	I	8.4E-02	I			2.4E-05	AC	8.4E-02	AC
Chloroethane (ethyl chloride)	75-00-3					1.0E+01	I				
Chloroform	67-66-3	1.0E-02	I			1.0E-01	A				
Chloromethane (methyl chloride)	74-87-3			1.3E-02	H	9.0E-02	I	1.8E-06	H	6.3E-03	calc
Chlorophenol, 2-	95-57-8	5.0E-03	I			1.4E-03	AC				

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Chloropropene, 3- (allyl chloride)	107-05-1					1.0E-03	I	6.0E-06	C99a	2.1E-02	calc
Chromium (III)	16065-83-1	1.5E+00	I								
Chromium (VI)	18540-29-9	3.0E-03	I								
Chrysene	218-01-9			1.2E-01	C99a			1.1E-05	C99a	3.9E-02	calc
Cobalt	7440-48-4	2.0E-02	SF								
Copper	7440-50-8	(only a drinking water action level is available for this metal)									
Cresol, p-	106-44-5	5.0E-03	H			6.0E-01	surr (C00)				
Cresol, o-	95-48-7	5.0E-02	I			6.0E-01	surr (C00)				
Cresol, m-	108-39-4	5.0E-02	I			6.0E-01	surr (C00)				
Cresols (total)	1319-77-3	5.0E-02	surr (I)			6.0E-01	C00				
Cumene	98-82-8	1.0E-01	I			4.0E-01	I				
Cyclohexanol	108-93-0	1.7E-05	solv			2.0E-05	solv				
Cyclohexanone	108-94-1	5.0E+00	I								
DDD	72-54-8			2.4E-01	I						
DDE	72-55-9			3.4E-01	I						
DDT, p,p'-	50-29-3	5.0E-04	I	3.4E-01	I			9.7E-05	I	3.4E-01	calc
Di-n-butyl phthalate	84-74-2	1.0E-01	I								
Di-n-octyl phthalate	117-84-0	2.0E-02	H								
Diallate	2303-16-4			6.1E-02	H						
Dibenz{a,h}anthracene	53-70-3			7.3E+00	TEF			1.2E-03	C99a	4.2E+00	calc
Dibromo-3-chloropropane, 1,2-	96-12-8			1.4E+0	H	2.0E-04	I	6.9E-07	H	2.4E-03	calc

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Dichlorobenzene, 1,2-	95-50-1	9.0E-02	I			2.0E-01	H				
Dichlorobenzene, 1,4-	106-46-7			2.4E-2	H	8.0E-01	I	1.1E-05	C99a	3.9E-02	calc
Dichlorobenzidine, 3,3'-	91-94-1			4.5E-01	I			3.4E-04	C99a	1.2E+00	calc
Dichlorodifluoromethane (Freon 12)	75-71-8	2.0E-01	I			2.0E-01	H				
Dichloroethane, 1,2-	107-06-2			9.1E-2	I	2.4E+00	A	2.6E-05	I	9.1E-02	calc
Dichloroethane, 1,1-	75-34-3	1.0E-01	H			5.0E-01	H	1.6E-06	C99a	5.6E-03	calc
Dichloroethylene, 1,1-	75-35-4	9.0E-03	I	6.0E-1	I	7.0E-02	C00	5.0E-05	I	1.8E-01	calc
Dichloroethylene, *trans*-1,2-	156-60-5	2.0E-02	I								
Dichloroethylene, cis-1,2-	156-59-2	1.0E-02	H								
Dichlorophenol, 2,4-	120-83-2	3.0E-03	I								
Dichlorophenoxyacetic acid, 2,4- (2,4-D)	94-75-7	1.0E-02	I								
Dichloropropane, 1,2-	78-87-5	9.0E-02	A	6.8E-2	H	4.0E-03	I				
Dichloropropene, *trans*-1,3-	10061-02-6	3.0E-02	I	1.0E-1	I	2.0E-02	surr (I)	4.0E-06	surr (I)	1.4E-02	calc
Dichloropropene, *cis*-1,3-	10061-01-5	3.0E-02	I	1.0E-1	I	2.0E-02	surr (I)	4.0E-06	surr (I)	1.4E-02	calc
Dichloropropene, 1,3- (mixture of isomers)	542-75-6	3.0E-02	I	1.0E-01	I	2.0E-02	I	4.0E-06	I	1.4E-02	calc
Dieldrin	60-57-1	5.0E-05	I	1.6E+01	I			4.6E-03	I	1.6E+01	calc
Diethyl phthalate	84-66-2	8.0E-01	I								
Diethylstilbestrol	56-53-1			4.7E+03	H						
Dimethoate	60-51-5	2.0E-04	I								
Dimethoxybenzidine, 3,3'-	119-90-4			1.4E-02	H						
Dimethyl formamide, N,N- (DMF)	68-12-2	1.0E-01	H			3.0E-02	I				
Dimethylbenz{a}anthracene, 7,12-	57-97-6							7.1E-02	C99a	2.5E+02	calc

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Dimethylbenzidine, 3,3'-	119-93-7			9.2E+00	H						
Dimethylphenol, 2,4-	105-67-9	2.0E-02	I								
Dinitrobenzene, 1,3-	99-65-0	1.0E-04	I								
Dinitrophenol, 2,4-	51-28-5	2.0E-03	I								
Dinitrotoluene, 2,6-	606-20-2	1.0E-03	H	6.8E-01	surr (I)						
Dinitrotoluene, 2,4-	121-14-2	2.0E-03	I	6.8E-01	surr (I)			8.9E-05	C99a	3.1E-01	calc
Dioxane, 1,4-	123-91-1			1.1E-2	I	3.0E+00	C00	7.7E-06	C99a	2.7E-02	calc
Diphenylamine	122-39-4	2.5E-02	I								
Diphenylhydrazine, 1,2-	122-66-7			8.0E-1	I			2.2E-04	I	7.7E-01	calc
Disulfoton	298-04-4	4.0E-05	I								
Endosulfan (Endosulfan I and II,mixture)	115-29-7	6.0E-03	I								
Endrin	72-20-8	3.0E-04	I								
Epichlorohydrin	106-89-8	2.0E-03	H	9.9E-3	I	1.0E-03	I	1.2E-06	I	4.2E-03	calc
Epoxybutane, 1,2-	106-88-7					2.0E-02	I				
Ethoxyethanol acetate, 2-	111-15-9	3.0E-01	H			3.0E-01	C00				
Ethoxyethanol, 2-	110-80-5	4.0E-01	H			2.0E-01	I				
Ethyl acetate	141-78-6	9.0E-01	I								
Ethyl ether	60-29-7	2.0E-01	I								
Ethyl methacrylate	97-63-2	9.0E-02	H								
Ethyl methanesulfonate	62-50-0			2.9E+02	RQ						
Ethylbenzene	100-41-4	1.0E-01	I			1.0E+00	I	1.1E-06	SF	3.9E-03	calc
Ethylene oxide	75-21-8			1.0E+0	H	3.0E-02	C00	1.0E-04	H	3.5E-01	calc
Ethylene dibromide (1,2-dibromoethane)	106-93-4			8.5E+1	I	2.0E-04	H	2.2E-04	I	7.7E-01	calc
Ethylene glycol	107-21-1	2.0E+00	I			4.0E-01	C00				

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Ethylene thiourea	96-45-7	8.0E-05	I	1.1E-01	H			1.3E-05	C99a	4.6E-02	calc
Fluoranthene	206-44-0	4.0E-02	I								
Fluoride	16984-48-8	0.12	surr (I)								
Formaldehyde	50-00-0	2.0E-01	I			9.8E-03	A	1.3E-05	I	4.6E-02	calc
Formic acid	64-18-6	2.0E+00	H								
Furfural	98-01-1	3.0E-03	I			5.0E-02	H				
HCH, beta-	319-85-7			1.8E+00	I			5.3E-04	I	1.9E+00	calc
HCH, gamma- (Lindane)	58-89-9	3.0E-04	I	1.3E+00	H			3.1E-04	C99a	1.1E+00	calc
HCH, alpha-	319-84-6	8.0E-03	A	6.3E+00	I			1.8E-03	I	6.3E+00	calc
Heptachlor	76-44-8	5.0E-04	I	4.5E+00	I			1.3E-03	I	4.6E+00	calc
Heptachlor epoxide	1024-57-3	1.3E-05	I	9.1E+00	I			2.6E-03	I	9.1E+00	calc
Hexachloro-1,3-butadiene	87-68-3	3.0E-04	SF	7.8E-2	I			2.2E-05	I	7.7E-02	calc
Hexachlorobenzene	118-74-1	8.0E-04	I	1.6E+0	I			4.6E-04	I	1.6E+00	calc
Hexachlorocyclopentadiene	77-47-4	6.0E-03	I			2.0E-04	I				
Hexachlorodibenzo-p-dioxins (HxCDDs)	34465-46-8			1.56E+04	WHO98			3.3E+00	WHO98	1.5E+04	WHO98
Hexachlorodibenzofurans (HxCDFs)	55684-94-1			1.56E+04	WHO98			3.3E+00	WHO98	1.5E+04	WHO98
Hexachloroethane	67-72-1	1.0E-03	I	1.4E-02	I			4.0E-06	I	1.4E-02	calc
Hexachlorophene	70-30-4	3.0E-04	I								
Hexane, n-	110-54-3	1.1E+01	SF			2.0E-01	I				
Hydrogen Sulfide	7783-06-4	3.0E-03	I								
Indeno{1,2,3-cd}pyrene	193-39-5			1.2E+00	C99a			1.1E-04	C99a	3.9E-01	calc
Isobutyl alcohol	78-83-1	3.0E-01	I								
Isophorone	78-59-1	2.0E-01	I	9.5E-04	I	2.0E+00	C99b				
Kepone	143-50-0	5.0E-04	A								

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Lead	7439-92-1	(only a drinking water action level is available for this metal)									
Manganese	7439-96-5	4.7E-02	I								
Mercury	7439-97-6	1.0E-04	surr (I)			3.0E-04	I				
Methacrylonitrile	126-98-7	1.0E-04	I			7.0E-04	H				
Methanol	67-56-1	5.0E-01	I			4.0E+00	C00				
Methoxychlor	72-43-5	5.0E-03	I								
Methoxyethanol, 2-	109-86-4	1.0E-03	H			2.0E-02	I				
Methoxyethanol acetate, 2-	110-49-6	2.0E-03	H			9.0E-02	C00				
Methyl parathion	298-00-0	2.5E-04	I								
Methyl methacrylate	80-62-6	1.4E+00	I			7.0E-01	I				
Methyl isobutyl ketone	108-10-1	8.0E-02	H			8.0E-02	H				
Methyl ethyl ketone	78-93-3	6.0E-01	I			1.0E+00	I				
Methyl tert-butyl ether (MTBE)	1634-04-4					3.0E+00	I				
Methylcholanthrene, 3-	56-49-5							6.3E-03	C99a	2.2E+01	calc
Methylene bromide (dibromomethane)	74-95-3	1.0E-02	H								
Methylene Chloride (dichloromethane)	75-09-2	6.0E-02	I	7.5E-03	I	3.0E+00	H	4.7E-07	I	1.6E-03	calc
Molybdenum	7439-98-7	5.0E-03	I								
N-Nitroso-di-n-butylamine	924-16-3			5.4E+00	I			1.6E-03	I	5.6E+00	calc
N-Nitroso-di-n-propylamine	621-64-7			7.0E+00	I			2.0E-03	C99a	7.0E+00	calc
N-Nitrosodiethylamine	55-18-5			1.5E+02	I			4.3E-02	I	1.5E+02	calc
N-Nitrosodimethylamine	62-75-9	8.00E-06	SF	5.1E+01	I			1.4E-02	I	4.9E+01	calc
N-Nitrosodiphenylamine	86-30-6	2.00E-02	SF	4.9E-03	I			2.6E-06	C99a	9.1E-03	calc
N-Nitrosomethylethylamine	10595-95-6			2.2E+01	I			6.3E-03	C99a	3.7E+00	C99a

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
N-Nitrosopiperidine	100-75-4							2.7E-03	C99a	9.5E+00	calc
N-Nitrosopyrrolidine	930-55-2			2.1E+00	I			6.1E-04	I	2.1E+00	calc
Naphthalene	91-20-3	2.0E-02	I			3.0E-03	I				
Nickel	7440-02-0	2.0E-02	I								
Nitrobenzene	98-95-3	5.0E-04	I			2.0E-03	H				
Nitropropane, 2-	79-46-9					2.0E-02	I	2.7E-03	H	9.5E+00	calc
Octamethyl pyrophosphoramide	152-16-9	2.0E-03	H								
Parathion (ethyl)	56-38-2	6.0E-03	H								
Pentachlorobenzene	608-93-5	8.0E-04	I								
Pentachlorodibenzo-p-dioxins (PeCDDs)	36088-22-9			1.56E+05	WHO98			3.3E+01	WHO98	1.5E+05	WHO98
Pentachlorodibenzofurans (PeCDFs)	30402-15-4			7.8E+04	WHO98			1.7E+01	WHO98	7.5E+04	WHO98
Pentachloronitrobenzene (PCNB)	82-68-8	3.0E-03	I	2.6E-01	H						
Pentachlorophenol	87-86-5	3.0E-02	I	1.2E-01	I			5.1E-06	C99a	1.8E-02	calc
Phenol	108-95-2	6.0E-01	I			2.0E-01	C00				
Phenyl mercuric acetate	62-38-4	8.0E-05	I								
Phenylenediamine, 1,3-	108-45-2	6.0E-03	I								
Phorate	298-02-2	2.0E-04	H								
Phthalic anhydride	85-44-9	2.0E+00	I			1.2E-01	H				
Polychlorinated biphenyls (Aroclors)	1336-36-3	2.0E-05	surr (I)	4.0E-01	I			1.0E-04	I	4.0E-01	I
Pronamide	23950-58-5	7.5E-02	I								
Propylene oxide (1,2-epoxypropane)	75-56-9			2.4E-01	I	3.0E-02	I	3.7E-06	I	1.3E-02	calc

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Pyrene	129-00-0	3.0E-02	I								
Pyridine	110-86-1	1.0E-03	I			7.0E-03	EPA86				
Safrole	94-59-7			1.8E-01	RQ						
Selenium	7782-49-2	5.0E-03	I								
Silver	7440-22-4	5.0E-03	I								
Strychnine and salts	57-24-9	3.0E-04	I								
Styrene	100-42-5	2.0E-01	I			1.0E+00	I				
Tetrachlorobenzene, 1,2,4,5-	95-94-3	3.0E-04	I								
Tetrachlorodibenzo-p-dioxin, 2,3,7,8-(2,3,7,8-TCDD)	1746-01-6			1.56E+05	DA85			3.3E+01	H	1.5E+05	H
Tetrachlorodibenzofuran, 2,3,7,8- (2,3,7,8-TCDF)	51207-31-9			1.56E+04	WHO98			3.3E+00	WHO98	1.5E+04	WHO98
Tetrachloroethane, 1,1,2,2-	79-34-5	6.0E-02	SF	2.0E-01	I			5.8E-05	I	2.0E-01	calc
Tetrachloroethane, 1,1,1,2-	630-20-6	3.0E-02	I	2.6E-02	I			7.4E-06	I	2.6E-02	calc
Tetrachloroethylene	127-18-4	1.0E-02	I	5.2E-02	HAD	3.0E-01	A	5.8E-07	HAD	2.0E-03	HAD
Tetrachlorophenol, 2,3,4,6-	58-90-2	3.0E-02	I								
Tetraethyl dithiopyrophosphate (Sulfotep)	3689-24-5	5.0E-04	I								
Thallium	7440-28-0	8.0E-05	surr (I)								
Thiram (Thiuram)	137-26-8	5.0E-03	I								
Toluene	108-88-3	2.0E-01	I			4.0E-01	I				
Toluenediamine, 2,4-	95-80-7			3.2E+00	H			1.1E-03	C99a	3.9E+00	calc
Toluidine, o-	95-53-4			2.4E-01	H			6.9E-05	AC	2.4E-01	AC
Toluidine, p-	106-49-0			1.9E-01	H						
Toxaphene (chlorinated camphenes)	8001-35-2			1.1E+00	I			3.2E-04	I	1.1E+00	calc

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Tribromomethane (bromoform)	75-25-2	2.0E-02	I	7.9E-03	I			1.1E-06	I	3.9E-03	calc
Trichloro-1,2,2-trifluoroethane, 1,1,2-	76-13-1	3.0E+01	I			3.0E+01	H				
Trichlorobenzene, 1,2,4-	120-82-1	1.0E-02	I			2.0E-01	H				
Trichloroethane, 1,1,1-	71-55-6	2.8E-01	SF			2.2E+00	SF				
Trichloroethane, 1,1,2-	79-00-5	4.0E-03	I	5.7E-02	I			1.6E-05	I	5.6E-02	calc
Trichloroethylene (1,1,2-trichloroethylene)	79-01-6			1.1E-02	HAD	6.0E-01	C00	1.7E-06	HAD	6.0E-03	HAD
Trichlorofluoromethane (Freon 11)	75-69-4	3.0E-01	I			7.0E-01	H				
Trichlorophenol, 2,4,5-	95-95-4	1.0E-01	I								
Trichlorophenol, 2,4,6-	88-06-2			1.1E-02	I			3.1E-06	I	1.1E-02	calc
Trichlorophenoxy)propionic acid, 2-(2,4,5- (Silvex)	93-72-1	8.0E-03	I								
Trichlorophenoxyacetic acid, 2,4,5-	93-76-5	1.0E-02	I								
Trichloropropane, 1,2,3-	96-18-4	6.0E-03	I	7.0E+00	H	5.0E-03	SF				
Triethylamine	121-44-8					7.0E-03	I				
Trinitrobenzene, sym- (1,3,5-Trinitrobenzene)	99-35-4	3.0E-02	I								
Tris(2,3-dibromopropyl)phosphate	126-72-7			9.8E+00	RQ						
Vanadium	7440-62-2	7.0E-03	H								
Vinyl acetate	108-05-4	1.0E+00	H			2.0E-01	I				
Vinyl chloride	75-01-4	3.0E-03	I	7.2E-01	I	1.0E-01	I	4.4E-06	I	1.5E-02	calc
Xylene, p-	106-42-3	2.0E+00	surr (H)			4.0E-01	surr (A)				

Table E-3. Human Health Benchmark Values (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per µg/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
Xylene, m-	108-38-3	2.0E+00	H			4.0E-01	surr (A)				
Xylene, o-	95-47-6	2.0E+00	H			4.0E-01	surr (A)				
Xylenes (total)	1330-20-7	2.0E+00	I			4.0E-01	A				
Zinc	7440-66-6	3.0E-01	I								

Key:

CASRN = Chemical Abstract Service registry number.
CSFo = oral cancer slope factor.
CSFi = inhalation cancer slope factor.
RfD = reference dose.
RfC = reference concentration.
URF = unit risk factor.

[a] Sources:
A = ATSDR MRLs (ATSDR, 2001)
AC = developed for the Air Characteristic Study (U.S. EPA, 1999g)
calc = calculated

C99a = CalEPA cancer potency factor (CalEPA, 1999a)
C99b = CalEPA chronic REL (CalEPA, 1999b)
C00 = CalEPA chronic REL (CalEPA, 2000)
DA85 = Dioxin Assessment (U.S. EPA, 1985)

EPA86 = Pyridine Health Effects Profile (U.S. EPA, 1986b)
HAD = Health Assessment Document (U.S. EPA, 1986a, 1987)

H = HEAST (U.S. EPA, 1997)
I = IRIS (U.S. EPA, 2001a)
RQ = reportable quantity adjustments (U.S. EPA, 1998d,e,f)
SF = Superfund Risk Issue Paper (U.S. EPA, 1998a,b; 1999a,b,c,d,e,f; 2000, 2001b,c,d)
solv = 63 FR 64371-0402 (U.S. EPA, 1998c)
surr = surrogate (source in parentheses; see section C.2.8)
TEF = toxicity equivalency factor (U.S. EPA, 1993)
WHO98 = World Health Organization (WHO) 1998 toxicity equivalency factor scheme (Van den Berg et al., 1998)

E-3.2.1 Benzene

The cancer risk estimates for benzene are provided as ranges in IRIS. The oral CSF for benzene is 1.5E-02 to 5.5E-02 $(mg/kg/d)^{-1}$ and the inhalation URF is 2.2E-06 to 7.8E-06 $(\mu g/m^3)^{-1}$ (U.S. EPA, 2001a). For IWEM, the upper range estimates were used (i.e., 5.5E-02 $(mg/kg/d)^{-1}$ and 7.8E-06 $(\mu g/m^3)^{-1}$ for the oral CSF and inhalation URF, respectively).

E-3.2.2 Vinyl Chloride

Based on use of the linearized multistage model, IRIS recommends an oral CSF of 7.2E-1 per mg/kg-d for vinyl chloride to account for continuous lifetime exposure during adulthood; this value was used in the IWEM tool.[1] Based on use of the linearized multistage model, an inhalation URF of 4.4E-6 per $\mu g/m^3$ to account for continuous, lifetime exposure during adulthood was recommended for vinyl chloride and was used for IWEM; an inhalation CSF of 1.5E-2 per mg/kg-d was calculated from the URF.[2]

E-3.2.3 Polychlorinated Biphenyls

There are two inhalation CSFs available from IRIS for polychlorinated biphenyls (PCBs): 0.4 per mg/kg-d for evaporated congeners and 2.0 per mg/kg-d for dust or aerosol (high risk and persistence). The inhalation CSF for evaporated congeners was used for IWEM.

E-3.2.4 Dioxin-like Compounds

Certain polychlorinated dibenzodioxin, polychlorinated dibenzofuran, and polychlorinated biphenyl (PCB) congeners are said to have "dioxin-like" toxicity, meaning that they are understood to have toxicity similar to that of 2,3,7,8-tetrachlorodibenzo(p)dioxin (2,3,7,8-TCDD). Although EPA has not developed health benchmarks for each specific compound with dioxin-like toxicity, these compounds have been assigned individual "toxicity equivalency factors" (TEFs; Van den Berg et al., 1998). TEFs are estimates of the toxicity of dioxin-like compounds relative to the toxicity of 2,3,7,8-TCDD, which is assigned a TEF of 1.0. TEF estimates are based on a

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[1] A twofold increase of the oral CSF to 1.4 per mg/kg-d to account for continuous lifetime exposure from birth was also recommended but was not used for IWEM.

[2] A twofold increase to 8.8E-6 per $\mu g/m^3$ for the inhalation URF, to account for continuous lifetime exposure from birth, was also recommended but was not used for IWEM.

knowledge of a constituent's mechanism of action, available experimental data, and other structure-activity information. We used the TEFs to calculate cancer slope factors for the dioxin and furan congeners (and congener groups) in the IWEM tool.

The dioxin-like congeners (and groups of congeners) included in IWEM are as follows:

- 2,3,7,8-TCDD,
- 2,3,7,8-Tetrachlorodibenzofuran (2,3,7,8-TCDF)
- Pentachlorodibenzodioxins (PeCDDs)
- Pentachlorodibenzofurans (PeCDFs)
- Hexachlorodibenzodioxins (HxCDDs)
- Hexachlorodibenzofurans (HxCDFs).

2,3,7,8-TCDF has a TEF of 0.1. The dioxin-like PeCDD congener is 1,2,3,7,8-PeCDD, which has a TEF of 1.0. The dioxin-like PeCDF congeners include 1,2,3,7,8-PeCDF and 2,3,4,7,8-PeCDF which have TEFs of 0.05 and 0.5, respectively. The dioxin-like HxCDD congeners include 1,2,3,7,8,9-HxCDD, 1,2,3,4,7,8-HxCDD, and 1,2,3,6,7,8-HxCDD, which have TEFs of 0.1. The dioxin-like HxCDF congeners include 1,2,3,7,8,9-HxCDF, 1,2,3,4,7,8-HxCDF, 1,2,3,6,7,8-HxCDF, and 2,3,4,6,7,8-HxCDF, which also have TEFs of 0.1. Table E-4 shows the TEFs that we used to calculate CSFs for the dioxin and furan congeners (and congener groups) for the purpose of developing HBNs for the Tier 1 tool.

Table E-4. TEFs Used for Dioxin and Furan Congeners

Constituent Name	TEF	CSFo $(\text{mkd})^{-1}$	CSFo Source	URF $(\mu g/m^3)^{-1}$	URF Source	CSFi $(\text{mkd})^{-1}$	CSFi Source
Dioxins							
Pentachlorodibenzodioxins	1	1.56+05	WHO 1998	3.3E+01	WHO 1998	1.56+05	WHO 1998
2,3,7,8-TCDD	1	1.56+5	EPA, 1985	3.3E+01	EPA, 1997	1.56+5	EPA, 1985
Hexachlorodibenzodioxins	0.1	1.56+4	WHO 1998	3.3E+00	WHO 1998	1.56+4	WHO 1998
Furans							
Hexachlorodibenzofurans	0.1	1.56+4	WHO 1998	3.3E+00	WHO 1998	1.56+4	WHO 1998
Pentachlorodibenzofurans	0.5	7.8+4	WHO 1998	1.7E+01	WHO 1998	7.8+4	WHO 1998
2,3,7,8-TCDF	0.1	1.56+4	WHO 1998	3.3E+00	WHO 1998	1.56+4	WHO 1998

WHO 98 = TEFs presented in Van den Berg et al. (1998)
EPA, 1997 = HEAST (U.S. EPA, 1997).

The human health benchmarks calculated using the TEFs for 1,2,3,4,7,8-hexachlorodibenzo-p-dioxin and 1,2,3,4,7,8-hexachlorodibenzofuran were surrogates for hexachlorodibenzo-p-dioxins (HxCDDs) and hexachlorodibenzofurans (HxCDFs), respectively. The human health benchmarks for 1,2,3,7,8-pentachlorodibenzo-p-dioxin and 2,3,4,7,8-pentachlorodibenzofuran were used to represent pentachlorodibenzodioxins (PeCDDs) and pentachlorodibenzofurans (PeCDFs), respectively. The human health benchmarks for 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD) and 2,3,7,8-tetrachlorodibenzofuran were used to represent tetrachlorodibenzo-p-dioxins (TCDDs) and tetrachlorodibenzofurans (TCDFs), respectively. When TEFs varied within a class of dioxin-like compounds (i.e., pentachlorodibenzofurans), the TEF most protective of human health was used.

E-3.2.5 Superfund Technical Support Center Provisional Benchmarks

Table E-5 lists the provisional human health benchmarks from the Superfund Technical Support Center that were used for some of the IWEM constituents. A provisional subchronic RfC of 2.0E-2 mg/m^3 was developed by the Superfund Technical Support Center (U.S. EPA, 1999a) for carbon tetrachloride; a provisional chronic RfC of 7.0E-3 mg/m^3 was derived from this value by applying an uncertainty factor of 3 to account for the use of a subchronic study.

Table E-5. Provisional Human Health Benchmarks Developed by the Superfund Technical Support Center

CASRN	Chemical Name	Benchmark Type	Benchmark Value	Units	Reference
108-90-7	Chlorobenzene	RfC	6.0E-02	mg/m^3	U.S. EPA, 1998a
7440-48-4	Cobalt (and compounds)	RfD	2.0E-02	mg/kg-d	U.S. EPA, 2001b
100-41-4	Ethylbenzene	URF	1.1E-06	$(\mu g/m3)^{-1}$	U.S. EPA, 1999b
87-68-3	Hexachlorobutadiene	RfD	3.0E-04	mg/kg-d	U.S. EPA, 1998b
110-54-3	Hexane	RfD	1.1E+01	mg/kg-d	U.S. EPA, 1999c
62-75-9	N-Nitrosodimethylamine (N-methyl-N-nitroso-methanamine)	RfD	8.0E-06	mg/kg-d	U.S. EPA, 2001c
86-30-6	N-Nitrosodiphenylamine	RfD	2.0E-02	mg/kg-d	U.S. EPA, 2001d
79-34-5	Tetrachloroethane, 1,1,2,2-	RfD	6.0E-02	mg/kg-d	U.S. EPA, 2000
71-55-6	Trichloroethane, 1,1,1-	RfD	2.8E-01	mg/kg-d	U.S. EPA, 1999d
71-55-6	Trichloroethane, 1,1,1-	RfC	2.2E+00	mg/m^3	U.S. EPA, 1999e
96-18-4	Trichloropropane, 1,2,3-	RfC	5.0E-03	mg/m^3	U.S. EPA, 1999f

E-3.2.6 Benchmarks From Other EPA Sources

For some IWEM constituents, human health benchmarks were not available from IRIS, the Superfund Technical Support Center, HEAST, ATSDR, or CalEPA, but were available from other EPA sources:

- The provisional oral CSF of 5.2E-2 per mg/kg-d, provisional inhalation URF of 5.8E-7 per µg/m^3, and the provisional inhalation CSF of 2.0E-3 per mg/kg-d developed for tetrachloroethylene by EPA in a Health Assessment Document (HAD) (U.S. EPA, 1986a) were used.
- For trichloroethylene, provisional cancer benchmarks developed by EPA in a HAD (U.S. EPA, 1987) were used and include the oral CSF of 1.1E-2 per mg/kg-d, inhalation URF of 1.7E-6 per µg/m^3, and inhalation CSF of 6.0E-3 per mg/kg-d.
- A provisional RfD of 1.7E-5 mg/kg-d and a provisional RfC of 2.0E-5 mg/m^3 were derived for cyclohexanol in the final listing rule for solvents (63 FR 64371) and were used (U.S. EPA, 1998c).
- An acceptable daily intake (ADI) of 2.0E-03 mg/kg-d from inhalation (7.0E-3 mg/m^3) was identified for pyridine (U.S. EPA, 1986b).
- EPA calculated an oral cancer potency factor of 293 per mg/kg-d for ethyl methanesulfonate in a reportable quantity adjustment evaluation (U.S. EPA, 1998d).
- EPA calculated an oral cancer potency factor of 0.18 per mg/kg-d for safrole in a reportable quantity adjustment evaluation (U.S. EPA, 1998e).
- EPA calculated an oral cancer potency factor of 9.8 per mg/kg-d for tris(2,3-dibromopropyl)phosphate in a reportable quantity adjustment evaluation (U.S. EPA, 1998f).
- The cancer slope factor for dibenzo(a,h)anthracene was calculated using a TEF approach developed for polycyclic aromatic hydrocarbons (U.S. EPA, 1993). The TEF approach assigns dibenzo(a,h)anthracene a TEF of 1 relative to the toxicity of benzo(a)pyrene. The oral CSF for dibenzo(a,h)anthracene is therefore the same as the IRIS (U.S. EPA, 2001a) value for benzo(a)pyrene: 7.3.E+00 $(mg/kg\text{-}d)^{-1}$.

E-3.2.7 Air Characteristic Study Provisional Benchmarks

Provisional inhalation health benchmarks were developed in the Air Characteristic Study (U.S. EPA, 1999g) for several constituents lacking IRIS, HEAST, alternative EPA, or ATSDR values. For 2-chlorophenol, a provisional RfC was developed using route-to-route extrapolation of the oral RfD. Using route-to-route extrapolations based on oral CSFs from IRIS and HEAST, the Air Characteristic Study developed provisional inhalation URFs and inhalation CSFs for bromodichloromethane, chlorodibromomethane, and o-Toluidine.

These provisional inhalation benchmark values are summarized in Table E-6 below. Additional details on the derivation of these inhalation benchmarks can be found in the *Revised Risk Assessment for the Air Characteristic Study* (U.S. EPA, 1999g).

Table E-6. Provisional Inhalation Benchmarks Developed in the Air Characteristic Study

CASRN	Chemical Name	RfC (mg/m^3)	RfC Target Effect	URF (µg/m^3)$^{-1}$	CSFi (mg/kg-d)$^{-1}$
75-27-4	Bromodichloromethane (dichlorobromomethane)			1.8E-05	6.2E-02
124-48-1	Chlorodibromomethane (dibromochloromethane)			2.4E-05	8.4E-02
95-57-8	2-Chlorophenol (o-)	1.4E-03	Reproductive, developmental		
95-53-4	o-Toluidine (2-methylaniline)			6.9E-05	2.4E-01

E-3.2.8 Surrogate Health Benchmarks

For several IWEM constituents, IRIS benchmarks for similar chemicals were used as surrogate data. The rationale for these recommendations is as follows:

- cis-1,3-Dichloropropylene and trans-1,3-dichloropropylene were based on 1,3-dichloropropene. The studies cited in the IRIS file for 1,3-dichloropropene used a technical-grade chemical that contained about a 50/50 mixture of the cis- and trans-isomers. The RfD is 3E-02 mg/kg-d and the RfC is 2E-02 mg/m^3. The oral CSF for 1,3-dichloropropene is 0.1 (mg/kg-d)$^{-1}$ and the inhalation URF is 4E-06 (µg/m^3)$^{-1}$.

- The IRIS oral CSF for the 2,4-/2,6-dinitrotoluene mixture (6.8E-01 per mg/kg-d) was used as the oral CSFs for 2,4-dinitrotoluene and 2,6-dinitrotoluene.

- The RfDs for o- and m-cresol (both 5E-02 mg/kg/d) are cited on IRIS. The provisional RfD for p-cresol (5E-03 mg/kg/d) is from HEAST. Cresol mixtures contain all three cresol isomers. Based on the hierarchy described above (i.e., IRIS is preferred over HEAST because IRIS is EPA's official repository of Agency-wide consensus human health risk information), the RfD for m-cresol (5E-02 mg/kg-d) was used as a surrogate for cresol mixtures.

- Fluoride was based on fluorine. The IRIS RfD for fluorine (0.12 mg/kg-d) is based on soluble fluoride and related to the endpoint of skeletal fluorisis.

- The RfD for methyl mercury (1E-04 mg/kg-d) was used as a surrogate for elemental mercury.

- The RfD for Arochlor 1254 (2E-05 mg/kg-d) was used as a surrogate for PCBs.

- Thallium was based on thallium chloride. There are several thallium salts that have RfDs in IRIS. The lowest value among the thallium salts (8E-05 mg/kg-d) is routinely used to represent thallium in risk assessments.

- p-Xylene was based on total xylenes. An RfD of 2 mg/kg-d is listed for total xylenes, m-xylene, and o-xylene in IRIS. Total xylenes contain a mixture of all three isomers; therefore, the RfD likely is appropriate for p-xylene.

E-3.2.9 Chloroform

EPA has classified chloroform as a Group B2, Probable Human Carcinogen, based on an increased incidence of several tumor types in rats and mice (U.S. EPA, 2001a). However, based on an evaluation initiated by EPA's Office of Water (OW), the Office of Solid Waste (OSW) now believes the weight of evidence for the carcinogenic mode of action for chloroform does not support a mutagenic mode of action; therefore, a nonlinear low-dose extrapolation is more appropriate for assessing risk from exposure to chloroform. EPA's Science Advisory Board (SAB), the World Health Organization (WHO), the Society of Toxicology, and EPA all strongly endorse the nonlinear approach for assessing risks from chloroform.

Although OW conducted its evaluation of chloroform carcinogenicity for oral exposure, a nonlinear approach for low-dose extrapolation would apply to inhalation exposure to chloroform as well, because chloroform's mode of action is understood to be the same for both ingestion and inhalation exposures. Specifically, tumorigenesis for both ingestion and inhalation exposures is induced through cytotoxicity (cell death) produced by the oxidative generation of highly reactive metabolites (phosgene and hydrochloric acid), followed by regenerative cell proliferation (U.S. EPA, 1998g). Chloroform-induced liver tumors in mice have only been seen after bolus corn oil dosing and have not been observed following administration by other routes (i.e., drinking water and inhalation). As explained in EPA OW's March 31, 1998, and December 16, 1998, *Federal Register* notices pertaining to chloroform (U.S. EPA, 1998g and 1998h, respectively), EPA now believes that "based on the current evidence for the mode of action by which chloroform may cause tumorigenesis, ...a nonlinear approach is more appropriate for extrapolating low-dose cancer risk rather than the low-dose linear approach..."(U.S. EPA, 1998g). OW determined that, given chloroform's mode of carcinogenic action, liver toxicity (a noncancer health effect) actually "is a more sensitive effect of chloroform than the induction of tumors" and that protecting against liver toxicity "should be protective against carcinogenicity given that the putative mode of action understanding for chloroform involves cytotoxicity as a key event preceding tumor development" (U.S. EPA, 1998g).

The recent evaluations conducted by OW concluded that protecting against chloroform's noncancer health effects protects against excess cancer risk. EPA now believes that the noncancer health effects resulting from inhalation of chloroform would precede the development of cancer and would occur at lower doses than would tumor development. Although EPA has not finalized a noncancer health benchmark for inhalation exposure (i.e., an RfC), ATSDR has developed an inhalation MRL for chloroform. Therefore, ATSDR's chronic inhalation MRL for chloroform (0.1 mg/m^3) was used in IWEM.

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