

Input Parameter Values for the Industrial D Tier 1 Tool

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**United States Environmental Protection Agency
Office of Solid Waste
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1.0 INTRODUCTION

The U.S. Environmental Protection Agency's (EPA's or USEPA's) Office of Solid Waste (OSW) is developing the ***Guide for Industrial Waste Management*** to facilitate evaluation of non-hazardous industrial waste management alternatives. One aspect of the guidance is a three-tiered groundwater modeling framework designed to determine if waste management unit (WMU) designs are protective of groundwater resources. The degree of groundwater protection provided by a particular design is determined by modeling the migration of waste constituents from the WMU through the subsurface to a monitoring point in an aquifer. The tiered approach was chosen to provide facility managers, the public, and state regulators flexibility in assessing the protectiveness of particular WMU designs.

A Tier 1 evaluation (the most protective analysis) consists of using a tabulated list of the maximum recommended leachate concentrations (or Leachate Concentration Threshold Values, LCTVs) to compare against the expected leachate concentrations from the WMU of concern. The Tier 1 LCTV tables are compilations of probabilistic groundwater fate and transport modeling results conducted with EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP). EPACMTP simulates subsurface fate and transport of contaminants leaching from the bottom of a waste management unit and predicts concentrations of those contaminants in a downgradient groundwater well. In making these predictions, the model quantitatively accounts for many complex processes that serve to dilute and attenuate the concentrations of waste constituents as they move through the subsurface to the well.

This report is organized as follows: The input parameter values that we will use in the Tier 1 EPACMTP modeling are presented in four tables (one each for surface impoundments, landfills, waste piles, and land application units) in Section 2. Section 3 presents the maximum contaminant levels (MCLs) and health-based numbers (HBNs) that we will use to establish protective contaminant concentrations in the modeled downgradient groundwater well. Attachments A, B, and C provide, respectively, the equations for the shower model (discussed in Section 3), the contaminant-specific parameter values used in the shower model, and the human health benchmarks used in developing the revised Tier 1 tool.

2.0 EPACMTP INPUT PARAMETER VALUES FOR THE TIER 1 TOOL

This section provides the input parameters that we are using in our EPACMTP model for the purpose of developing the Tier 1 LCTVs. Section 2.1 outlines the most important changes we made to the Tier 1 parameters since developing the draft (1999) Tier 1 tool. Section 2.2 provides tables of the EPACMTP input parameter values for the Tier 1 tool. Section 2.3 provides references for this section.

2.1 Most Important Changes to the Model Parameter Values for the Tier 1 Tool

The Background Document for the Industrial Waste Management Evaluation Model (IWEM) (USEPA, 1999) provides the parameter values that we used with the EPACMTP model to develop the draft Tier 1 tool. The following sections briefly describe the major changes we are making to the Tier 1 parameter values in developing the revised Tier 1 tool.

2.1.1 New Surface Impoundment Database

For the revised Tier 1 tool, we are updating Tier 1 EPACMTP model input parameters to incorporate data that we collected to support our recently completed “Surface Impoundment Study” (USEPA, 2001). The Surface Impoundment Study is the product of a national survey of facilities that operate non-hazardous industrial waste surface impoundments. We used information in the Surface Impoundment Study to create a new database of surface impoundment characteristics that replaces an earlier database developed using the responses to EPA’s 1986 survey of Industrial D facilities (USEPA, 1986). The surface impoundment parameters that we are using from the Surface Impoundment Study include the following:

- Impoundment location (and associated climate, soil, and aquifer characteristics);
- Impoundment area;
- Ponding depth of water in the surface impoundment;
- Depth of base of the impoundment below ground surface;
- Operational life of the impoundment; and
- Proximity of the impoundment to a surface water body.

2.1.2 Revised Infiltration Rates for Unlined and Single (Compacted Clay)-Lined Surface Impoundments

To develop the revised version of the Tier 1 tool, EPACMTP will calculate infiltration rates for unlined and single (clay)-lined surface impoundments using an updated surface impoundment source module. We received public comment on the Industrial D tool that questioned the way that we modeled the saturated condition of the surface impoundment liner. In response to this comment, we revised the surface impoundment source module so that the clay liner is simulated as variably

saturated, rather than fully saturated. In addition, since the development of the draft Tier 1 tool, we have refined the way that we model the physical characteristics of surface impoundments. Specifically, the new surface impoundment module simulates the presence of a sludge layer in the impoundment. In addition, the module now simulates the presence of a zone beneath the unlined surface impoundment where the natural (native) subsurface material is clogged with solids that have migrated from the impoundment. Both of these features impede the migration of leachate from the surface impoundment to the unsaturated zone, reducing infiltration from the surface impoundment.

2.1.3 Revised Infiltration Rates for Unlined Waste Piles

As described in the Background Document for the Industrial Waste Management Evaluation Model (IWEM) (USEPA, 1999), to develop the Tier 1 tool, EPA used the Hydrologic Evaluation for Landfill Performance (HELP) model to estimate infiltration through unlined and single-lined waste piles. To account for the fact that waste type can influence infiltration through a waste pile, we assumed that the wastes managed in *single-lined* waste piles alternately could consist of relatively high permeability copper slags, relatively moderate permeability coal bottom ash, or relatively low permeability coal fly ash. However, we assumed that only the relatively moderate permeability coal bottom ash was managed in *unlined* waste piles. In the revised Tier 1 tool we will eliminate this inconsistency in how we calculate infiltration through single-lined and unlined waste piles. Specifically, we have new infiltration rates for unlined waste piles that are based on all three waste types that we considered in developing infiltration rates for single-lined waste piles. Table 2-4 (at the end of Section 2.2) presents the new infiltration rates for unlined waste piles.

2.1.4 Revised Infiltration Rates for Composite-Lined Landfills, Waste Piles, and Surface Impoundments

To develop the draft Tier 1 LCTVs, we used a single rate to quantify the infiltration of leachate through composite-lined landfills, surface impoundments, and waste piles (the infiltration rate for landfills and waste piles differed from the rate for impoundments). One peer reviewer of the draft Tier 1 tool felt that to be more consistent with the way that we probabilistically sample distributions of values for other important model parameters, we should evaluate a range of infiltration rates using actual data from studies, rather than evaluating only a single infiltration rate.

To support the development of revised infiltration rates for landfills, waste piles, and surface impoundments, we conducted an information collection effort that involved searching the available literature for data that quantify liner integrity and leachate infiltration through liners (Tetra Tech, 2001). We assembled these data and evaluated them for their applicability to the Industrial D Tier 1 tool. Our use of these data in developing revised infiltration rates is described below.

2.1.4.1 Composite-Lined Landfills and Waste Piles

To develop the draft (1999) Tier 1 LCTVs for composite-lined landfills and waste piles, we calculated leakage through a single hole in a composite liner using the following equation developed by Bonaparte, et al. (1989):

$$Q = 0.21a^{0.1}h^{0.9}k_s^{0.74}$$

where:

- Q = steady-state rate of leakage through one hole in the liner (units of volume per time)
- a = area of hole in the geomembrane (units of area)
- h = head of liquid on top of geomembrane (units of length)
- k_s = hydraulic conductivity of the low-permeability soil (for example, clay) underlying the geomembrane (units of length per time)

This equation is applicable to cases where there is good contact between the geomembrane and the underlying compacted clay liner. We assumed that the area of the hole in the geomembrane was 0.005 in², the head on the liner was 1 foot, and the hydraulic conductivity of the clay liner was 1x10⁻⁷ centimeters/second (cm/sec). We based our estimate of the area of the hole on the work of Giroud and Bonaparte (1989), who, upon interviewing quality assurance personnel, concluded that a seam defect that may exist in a liner after intensive quality assurance would be equivalent to a hole with maximum diameter of approximately 0.04 to 0.12 inches (in; 0.001 to 0.01 in²). To calculate the infiltration rate per area of landfill (volume of leachate per area per time), we multiplied the calculated leakage through one hole (Q, above) by an estimated leak density of one hole per acre. We based our estimate of leak density on Giroud and Bonaparte's (1989) analysis of six case studies.

For the revised Tier 1 LCTVs, we are improving our method for estimating landfill and waste pile composite liner infiltration rates. For composite-lined landfills and waste piles, we developed a distribution of actual leak detection system (LDS) flow rates reported for geomembrane/geosynthetic clay composite-lined landfill cells constructed with formal construction quality assurance (CQA) programs. In generating the revised Tier 1 LCTVs, the EPACMTP model will randomly select infiltration rates from this distribution of LDS flow rates, rather than using only the single infiltration rate developed to generate the draft LCTVs.

Our new distribution of landfill and waste pile infiltration rates, summarized in Table 2-3 (presented at the end of Section 2.2), is based on monthly average LDS flow rates for 22 operating

landfill cells and 5 closed landfill cells¹. We compiled these data from Eith and Koerner (1997) and USEPA (1998). We included data for both operating and closed landfill cells in our distribution. We rejected the idea of including LDS flow rates for geomembrane/compacted clay composite-lined landfill cells in our distribution. For compacted clay liners (including composite geomembrane/compacted clay liners), consolidation water can be a large contributor to LDS flow, such that it is very difficult to determine how much of the LDS flow is due to liner leakage how much is due to clay consolidation. We also rejected LDS flow rates from three geomembrane/geosynthetic clay lined-cells that we felt were questionable. LDS flow rates for one cell were reported in USEPA (1998). Flow rate data were available for the cell's operating period and the cell's post-closure period. The average flow rate for the cell was 26 liters/hectare/day when the cell was operating and 59 liters/hectare/day when the cell was closed. We believe these flow rates, which were among the highest reported, are suspect because the flow rate from the closed cell was over twice the flow rate from the open cell, a pattern inconsistent with the other open cell/closed cell data pairs we reviewed. The other two rejected flow rates were reported in Tedder (1997). We rejected the Tedder (1997) values because flow rates for presumably the same cells were reported differently in two separate tables presented in the paper. Communication with the author revealed that he had adjusted some of his data to attempt to account for the effects of construction water.

2.1.4.2 Composite-Lined Surface Impoundments

To develop the draft (1999) Tier 1 LCTVs for composite-lined surface impoundments, we calculated infiltration rates using Bonaparte et al.'s (1989) equation presented in Section 2.1.4.1. We also used the same values for the variables in the equation that we used to develop the draft Tier 1 LCTVs for landfills and waste piles, except that we assumed that the head of liquid in surface impoundments (the depth of ponding) is 10 feet, rather than 1 foot.

For the revised Tier 1 LCTVs, we are enhancing our method for estimating surface impoundment composite liner infiltration rates. We are using the Bonaparte equation, as we did to calculate surface impoundment infiltration rates for the draft Tier 1 tool, but are improving how we develop the values of the variables in the equation. In addition, we are calculating infiltration rates for composite-lined surface impoundments probabilistically. The probabilistic approach involves randomly sampling values for ponding depth (head) from the new Surface Impoundment Study database (discussed in Section 2.1.1) and randomly sampling values of leak density from a new database we developed as part of our data collection effort. We are going to use the randomly sampled values in the infiltration equation in conjunction with constant values for clay liner hydraulic conductivity and hole size. Our new distribution of leak density, summarized in Table 2-2 (at the end of Section 2.2), is compiled from 26 leak density values reported in Rollin et al. (1999), McQuade and Needham (1999),

¹ The sources we assembled provided post-closure LDS flow data for five landfill cells for which we also had LDS flow data for the operating period. That is, the five closed cells are the same as five of the open cells.

and Laine (1991) for liners installed with formal CQA programs. The leak size we will use in the Bonaparte equation, 6 millimeters squared (mm^2), is the middle of a range of hole sizes reported by Rollin et al. (1999), who found that 25 percent of holes were less than 2mm^2 , 50 percent of holes were 2 to 10mm^2 , and 25 percent of holes were greater than 10mm^2 . The hydraulic conductivity of the clay liner, 1×10^{-7} cm/sec, is the same value we used for clay liner conductivity when estimating infiltration to develop the draft Tier 1 tool.

2.2 Tables of the EPACMTP Parameter Values for the Tier 1 Tool

This section contains four tables that list the input parameter values that will be used in the Tier 1 groundwater modeling conducted to support EPA's ***Guide for Industrial Waste Management***. Table 2-2 presents the surface impoundment parameter values; Table 2.3 presents the landfill parameter values; Table 2-4 presents the waste pile parameter values; and Table 2-5 presents the land application unit parameter values. The tables are presented at the end of this section. The footnotes referenced in the tables follow the presentation of the tables.

For the Tier 1 groundwater modeling, the Agency will use a probabilistic, or Monte Carlo, approach that is similar to approaches the Agency has used in other contaminant transport analyses conducted to support national-scale regulatory and guidance development, and is similar to the approach that the Agency used to develop the draft (1999) Tier 1 LCTV tables. In a Monte Carlo analysis, an analyst can specify each input to the EPACMTP model as a derived value, a constant value, a statistical distribution of values, or an empirical distribution of values. When EPACMTP is run, the model generates a value for each input parameter, as follows: 1) for each input that is specified as a constant value, this value is always used; 2) for each derived parameter, the model calculates its value using other input values; and 3) for the inputs that are specified as distributions, the model randomly draws a value for each input parameter from the appropriate distribution. Once the model compiles one complete set of modeling input values, the model is executed, and the model records the input and output values. The model repeats this procedure thousands of times, creating a distribution of the resulting groundwater well concentrations (the model output). The advantage of the probabilistic approach is that it accounts for the variability (diversity of input parameter values) and uncertainty (degree of confidence that the input parameter values are representative of the true values) in the input parameter values by computing a distribution of groundwater well concentrations that are based on representative distributions of input parameters and reasonable and representative combinations of these input parameters.

The values presented in the tables this section are those that will be used in the revised Tier 1 modeling. A few EPACMTP inputs are set to constant values; however, most input parameters are either derived or specified as a distribution of values. For these inputs, the values shown in the tables are selected percentiles from the respective distributions of values that are generated when the model is run. That is, for each waste management unit scenario, a default modeling run was conducted to

generate these percentile values, a procedure required by the site-based methodology incorporated within the EPACMTP model. In a site-based Monte Carlo analysis, the modeling is conducted for a database of waste sites on the assumption that these sites are an adequate representation of the universe of possible waste sites in the U.S.; thus, the modeling results are then applicable nationwide. The site-based methodology, which generates EPACMTP input parameter values through the use of linked databases containing waste management unit characteristics, climate data, and hydrogeological conditions, preserves statistical correlations among the input parameters and incorporates screening methodologies to prevent unreasonable combinations of input parameter values.

For each waste management unit type, statistical sampling was used to create a database of sites that includes data on WMU size and location. The climatic region index and aquifer type index for each site were then added to this site database; these indices link the site database to databases containing infiltration rates and aquifer characteristics. These databases were then compiled into an auxiliary EPACMTP input file that contains the data required to run a site-based modeling analysis. For each Monte Carlo realization, EPACMTP selects a waste site from the database in the auxiliary input file. Given the waste site's geographic location: 1) the climatic region and the randomly-generated soil type are then used by the model to determine the recharge and infiltration rates of the site from the database of HELP-modeled rates; 2) the aquifer type is used to determine the hydrogeologic parameters for the site by selecting at random a set of aquifer characteristics from those available in the American Petroleum Institute (API) hydrogeologic database (API, 1989). If the chosen combination of input values fails any of several screening methodologies, these input values are discarded and another set is generated. Thus, it is only when these databases are used together, along with the screening methodologies, that the complete distribution of input values are generated, meaning that a default modeling run was required to generate the data in these tables.

As an example, EPACMTP generates a distribution of values for the soil bulk density using three databases of soil parameters; there is a database for each soil type containing a distribution of values for each soil input parameter. During a site-based Monte Carlo modeling run, the soil type is automatically varied according to the nationwide occurrence of these three soil types. Because the soil bulk density is set to a constant value for each of the three soil types (1.65 g/cm³ for silty clay loam, 1.60 g/cm³ for sandy loam, and 1.67 g/cm³ for silty clay loam), and the soil type is automatically varied during the Monte Carlo modeling run, the resulting distribution of bulk density values ranges from 1.60 to 1.67 g/cm³.

In reviewing the attached tables, please note the following:

- EPACMTP version 1.2, the current publicly distributed version of EPACMTP, was used to generate the input parameter distributions for the landfill, waste pile, and land application scenarios. However, the surface impoundment source module within the EPACMTP model has

been updated for use in this project. This updated version of EPACMTP (beta 2.0) was used to generate the input parameter distributions for the surface impoundment scenario.

- The values presented in the tables for the landfill, waste pile, and surface impoundment scenarios were generated with Monte Carlo modeling runs consisting of 10,000 model realizations. However, an unexpected problem was encountered in conducting the land application unit modeling; the model stopped execution after 6,557 realizations. As discussed above, version 1.2 of the EPACMTP model (the version that currently is available to the public) was used to perform this land application unit modeling. Version 1.2 was developed at a time when computer processing speeds made conducting Monte Carlo runs of more than 2,000 realizations time-prohibitive. Thus, this version of EPACMTP was not intended to be used for more than 2,000 realizations and was not tested in this manner. The EPACMTP model currently is being enhanced and updated for use in this project; this revised version of EPACMTP will be able to make modeling runs of 10,000 realizations for all WMU scenarios. However, for the purposes of presenting the values to be used in this modeling, the expected error associated with using 6,557 rather than 10,000 realizations for the land application unit scenario is expected to be minimal.
- Leachate concentration, although technically an EPACMTP input, is not included in the attached tables of Tier 1 input values since this is the value that is compared with the LCTVs in the Tier 1 Lookup tables. In the EPACMTP modeling runs conducted to produce the Tier 1 LCTV tables, we will use a default value for the leachate concentration.
- The chemical-specific properties that are EPACMTP inputs (organic carbon distribution coefficient and hydrolysis rate for organics; soil/water distribution coefficient or adsorption isotherm for metals) are not included in this table because we currently are compiling and updating these values so that they are consistent across all modeling tools provided with the **Guide**. A table of chemical properties will be added to this report as soon as we finalize these values.
- Unlike surface impoundments and waste piles which are considered to be temporary waste management facilities, landfills are considered to be permanent. We assume that the waste in the landfill continues to leach to the subsurface until it is depleted. For this reason, the leaching duration for the landfill scenario is derived as a function of the amount of waste disposed and the rate at which it is leached to the subsurface. As a result, leaching duration is not presented in the Tier 1 parameter tables for landfills.

Table 2-1 presents an explanation of the abbreviations used in the tables of input parameter values presented in Tables 2-2, 2-3, 2-4, and 2-5

Table 2-1. Abbreviations Used in the Tables of Input Parameter Values

Symbol	Units
m	meters
m/yr	meters per year
yr	year
1/m	1 per meter (the mathematical inverse of a meter)
g/cm ³	grams per centimeter ³
cm ³ /g	centimeter ³ per grams
1/yr	1 per year (the mathematical inverse of a year)
cm	centimeter
cm/sec	centimeters per second
leaks/ha	number of leaks per hectare
degrees C	degrees Centigrade
degrees	angular degrees (for instance, there are 90 degrees in a right angle)
standard pH units	- log [H ⁺] (the negative log of the activity of the hydrogen ion)

Table 2-2. Parameter Values for Surface Impoundments

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Source Parameters											
SS1	Area	Regional Site-Based	m	26.0	174	401	1,740	4,050	16,700	51,600	USEPA, 2001
SS2	Length	Derived	m	5.10	13.2	20.0	41.7	63.6	129	227	Derived
SS3	Width	Derived	m	5.10	13.2	20.0	41.7	63.6	129	227	Derived
SS5	Recharge Rate	Regional Site-Based	m/yr	1.80e-03	9.90e-33	4.65e-02	2.10e-01	2.43e-01	3.53e-01	4.56e-01	ABB, 1995 and USEPA, 1997b
SS6	Infiltration Rate (NO LINER)	Derived	m/yr	1.01e-03	2.39e-01	4.59e-01	9.80e-01	2.22	3.35	25.3	Derived
SS6	Infiltration Rate (SINGLE LINER)	Derived	m/yr	1.21x10 ⁻³	3.81x10 ⁻²	5.85x10 ⁻²	1.06e-01	1.52e-01	2.15e-01	6.37e-01	Derived
SS6	Infiltration Rate (COMPOSITE LINER)	Derived	m/yr	0	0	0	1.34e-05	1.34e-04	3.80e-04	4.01e-03	Derived
SS7	Wastewater Ponding Depth	Regional Site-Based	m	0.0100	0.150	0.940	1.81	2.85	3.89	10.1	USEPA, 2001
SS8	Single Clay Liner Thickness	Constant	m	0.914							Assumption
SS9	Single Clay Liner Conductivity	Constant	cm/sec	1.00e-07							Assumption
SS10	Operational Life (Leaching Duration)	Regional Site-Based	yr	13	14	50	50	50	50	50	USEPA, 2001
SS15	Depth of Unit Below Land Surface	Regional Site-Based	m	0.00	0.00	0.00	1.07	3.05	4.57	7.62	USEPA, 2001
SS16	Thickness of Sludge	Constant	m	0.2							Assumption
	Saturated Conductivity of Sludge ^{3, 4}	Derived	cm/sec	1.26e-07	1.27e-07	1.27e-07	1.28e-07	1.31e-07	1.48e-07	1.77e-07	Derived
SS21	Composite Liner Leak Density	Empirical	leaks/ha	0	0	0	0.915	3.34	4.77	12.5	TetraTech, 2001
SS22	Distance to Nearest Surface Water Body	Regional Site-Based	m	30	150	260	360	500	1,600	5,000	USEPA, 2001
	Total Impoundment Operating Depth ³	Derived	m	0.110	0.250	1.04	1.91	2.95	3.99	10.2	Derived
	Ratio of Saturated Conductivity of Clogged Soil to that of Native Material ³	Constant	unitless	0.1							Assumption
	Depth of Clogging (invasion of suspended sediment into native material) ³	Constant	m	0.5							Assumption

Table 2-2. Parameter Values for Surface Impoundments

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Unsaturated Zone Parameters											
US1	Saturated Hydraulic Conductivity	Based on soil type ²	m/yr	0.00306	0.302	0.972	4.50	47.7	314	2,480	Carsel and Parrish, 1988
US2	Moisture Retention Parameter (alpha)	Based on soil type ²	1/m	0.0755	0.493	0.754	1.27	3.47	8.51	20.4	Carsel and Parrish, 1988
US3	Moisture Retention Parameter (beta)	Based on soil type ²	unitless	1.01	1.17	1.22	1.28	1.68	1.94	2.49	Carsel and Parrish, 1988
US4	Residual Water Content	Based on soil type ²	unitless	0.0125	0.0552	0.0717	0.0838	0.0921	0.0985	0.115	Carsel and Parrish, 1988
US5	Saturated Water Content	Based on soil type ²	unitless	0.410	0.410	0.410	0.430	0.430	0.430	0.450	Carsel and Parrish, 1988
US6	Thickness of Unsaturated Zone	Regional Site-Based	m	0.457	1.83	3.32	6.10	13.7	27.4	610	API, 1989
US7	Dispersivity	Derived	m	0.0301	0.0603	0.0930	0.154	0.321	0.623	1.00	Gelhar, 1986; EPRI, 1985; USEPA, 1997a
US8	Percent Organic Matter	Based on soil type ²	unitless	0.00279	0.0309	0.0539	0.0993	0.177	0.305	2.44	Carsel and others, 1988
US9	Bulk Density	Based on soil type ²	g/cm ³	1.60	1.60	1.60	1.67	1.67	1.67	1.67	Carsel and others, 1988
US10	Soil/Water Distribution Coefficient	Derived	cm ³ /g	chemical-specific value							Derived
US11	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
US12	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
US13	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-2. Parameter Values for Surface Impoundments

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Saturated Zone Parameters											
AS1	Average Particle Diameter	Empirical	cm	4.01e-04	1.47e-03	5.49e-03	1.94e-02	4.11e-02	7.63e-02	2.11e-01	Shea, 1974
AS2	Aquifer Effective Porosity	Derived	unitless	0.0501	0.105	0.162	0.234	0.295	0.333	0.428	Davis, 1969; McWorter and Sunada, 1977
AS3	Aquifer Bulk Density	Derived	g/cm³	1.16	1.29	1.43	1.56	1.63	1.70	1.80	Freeze and Cherry, 1979
AS4	Aquifer Saturated Thickness	Regional Site-Based	m	0.305	3.05	6.10	12.2	22.9	61.0	914	API, 1989
AS5	Longitudinal Hydraulic Conductivity	Regional Site-Based	m/yr	3.15	31.5	145	764	4,420	17,700	7,350,000	API, 1989
AS6	Anisotropy Ratio	Constant	unitless	1							Assumption
AS7	Hydraulic Gradient	Regional Site-Based	unitless	1.00e-06	6.00e-04	2.00e-03	6.71e-03	1.45e-02	3.10e-02	4.37e-01	API, 1989
AS8	Seepage Velocity	Derived	m/yr	0.100	0.915	4.14	19.3	98.0	460	10,900	Derived
AS9	Retardation Factor	Derived	unitless	chemical-specific value							Derived
AS10	Longitudinal Dispersivity	Gelhar Empirical	m	0.100	1.19	3.56	9.06	28.2	92.6	317	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS11	Transverse Dispersivity	Gelhar Empirical	m	0.0125	0.149	0.445	1.13	3.53	11.6	39.6	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS12	Vertical Dispersivity	Gelhar Empirical	m	0.0100	0.0100	0.0223	0.0566	0.176	0.579	1.98	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS13	Temperature of Ambient Aquifer Water	Empirical	degrees C	7.50	12.5	12.5	12.5	17.5	22.5	27.5	Collins, 1925
AS14	Ambient Groundwater pH	Empirical	standard units	3.20	5.21	6.04	6.79	7.39	7.88	9.69	data from USEPA's STORET database, reported in USEPA, 1997a
AS15	Fraction of Organic Carbon	Johnson SB	unitless	8.58e-06	1.35e-04	2.35e-04	4.27e-04	7.93e-04	1.35e-03	1.34e-02	data from USEPA's STORET database, reported in USEPA, 1997a
AS16	Radial Distance of Well from Downgradient Edge of Waste Unit	Constant	m	150							Policy for Tier 1
AS17	Angle of Well Off Plume Centerline	Constant	degrees	0							Policy for Tier 1
AS20	Depth of Well Below Water Table	Uniform	m	0.00137	0.786	2.08	5.16	12.0	28.9	906	API, 1989
AS21	Soil/Water Distribution Coefficient	Derived	cm³/g	chemical-specific value							Derived
AS22	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
AS23	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
AS24	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-3. Parameter Values for Landfills

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Source Parameters											
SS1	Area	Regional Site-Based	m	40.5	809	3,720	13,500	60,700	149,000	3,120,000	USEPA, 1986 and 1997b
SS2	Length	Derived	m	6.36	28.5	61.0	116	246	386	1,770	Derived
SS3	Width	Derived	m	6.36	28.5	61.0	116	246	386	1,770	Derived
SS5	Recharge Rate	Regional Site-Based	m/yr	1.00e-05	2.26e-02	7.80e-02	1.47e-01	3.42e-01	4.56e-01	1.15	ABB, 1995 and USEPA, 1997b
SS6	Infiltration Rate (NO LINER)	Regional Site-Based	m/yr	1.00e-05	1.96e-02	6.86e-02	1.30e-01	3.08e-01	4.50e-01	1.08	ABB, 1995 and USEPA, 1997b
SS6	Infiltration Rate (SINGLE LINER)	Regional Site-Based	m/yr	1.00e-05	1.88e-02	3.50e-02	4.32e-02	4.77e-02	4.86e-02	5.26e-02	USEPA, 1999
SS6	Infiltration Rate (COMPOSITE LINER)	Empirical	m/yr	0	0	0	0	7.30e-05	1.78e-04	4.01e-04	TetraTech, 2001
SS11	Fraction of Landfill Occupied by Waste of Concern	Constant	unitless	1							Policy for Tier 1
SS12	Depth of Waste Disposal Facility	Regional Site-Based	m	0.510	0.890	1.32	2.59	4.09	6.19	10.1	USEPA, 1986 and 1997b
SS13	Waste Density ⁵	Empirical	g/cm ³	0.700	0.736	0.792	0.887	1.33	1.46	2.08	Schanz and Salhotra, 1992
SS15	Depth of Unit Below Land Surface	Constant	m	0							No data available
FS1	Ratio of Waste Concentration to Leachate Concentration	Constant	L/kg	10,000							Policy for Tier 1

Table 2-3. Parameter Values for Landfills

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Unsaturated Zone Parameters											
US1	Saturated Hydraulic Conductivity	Based on soil type ²	m/yr	0.00377	0.596	2.08	7.98	35.7	168	2,450	Carsel and Parrish, 1988
US2	Moisture Retention Parameter (alpha)	Based on soil type ²	1/m	0.129	0.605	0.933	1.55	2.76	6.09	21.8	Carsel and Parrish, 1988
US3	Moisture Retention Parameter (beta)	Based on soil type ²	unitless	1.04	1.20	1.26	1.37	1.53	1.83	2.46	Carsel and Parrish, 1988
US4	Residual Water Content	Based on soil type ²	unitless	0.0102	0.0493	0.0608	0.0744	0.0858	0.0939	0.114	Carsel and Parrish, 1988
US5	Saturated Water Content	Based on soil type ²	unitless	0.410	0.410	0.430	0.450	0.450	0.450	0.450	Carsel and Parrish, 1988
US6	Thickness of Unsaturated Zone	Regional Site-Based	m	0.305	1.52	3.05	5.33	14.0	30.5	610	API, 1989
US7	Dispersivity	Derived	m	0.0267	0.0534	0.0871	0.137	0.329	0.691	1.00	Gelhar, 1986; EPRI, 1985; USEPA, 1997a
US8	Percent Organic Matter	Based on soil type ²	unitless	5.98e-03	3.33e-02	5.67e-02	1.00e-01	1.74e-01	2.93e-01	1.74	Carsel and others, 1988
US9	Bulk Density	Based on soil type ²	g/cm ³	1.60	1.60	1.65	1.65	1.67	1.67	1.67	Carsel and others, 1988
US10	Soil/Water Distribution Coefficient	Derived	cm3/g	chemical-specific value							Derived
US11	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
US12	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
US13	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-3. Parameter Values for Landfills

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Saturated Zone Parameters											
AS1	Average Particle Diameter	Empirical	cm	4.00e-04	1.45e-03	5.35e-03	1.94e-02	4.09e-02	7.62e-02	2.11e-01	Shea, 1974
AS2	Aquifer Effective Porosity	Derived	unitless	0.0500	0.103	0.163	0.236	0.296	0.334	0.426	Davis, 1969; McWorter and Sunada, 1977
AS3	Aquifer Bulk Density	Derived	g/cm ³	1.16	1.29	1.43	1.56	1.63	1.70	1.80	Freeze and Cherry, 1979
AS4	Aquifer Saturated Thickness	Regional Site-Based	m	0.305	3.17	7.32	10.7	27.4	76.2	914	API, 1989
AS5	Longitudinal Hydraulic Conductivity	Regional Site-Based	m/yr	3.15	94.6	315	1,890	9,000	27,800	5,800,000	API, 1989
AS6	Anisotropy Ratio	Constant	unitless	1							Assumption
AS7	Hydraulic Gradient	Regional Site-Based	unitless	2.00e-06	1.00e-03	2.00e-03	5.70e-03	1.70e-02	3.30e-02	5.34e-01	API, 1989
AS8	Seepage Velocity	Derived	m/yr	0.100	2.16	8.63	41.9	220	1,080	10,800	Derived
AS9	Retardation Factor	Derived	unitless	chemical-specific value							Derived
AS10	Longitudinal Dispersivity	Gelhar Empirical	m	0.108	1.27	3.84	8.42	30.8	85.8	230	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS11	Transverse Dispersivity	Gelhar Empirical	m	0.0135	0.158	0.480	1.05	3.86	10.7	28.7	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS12	Vertical Dispersivity	Gelhar Empirical	m	0.00500	0.00791	0.0240	0.0526	0.193	0.536	1.44	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS13	Temperature of Ambient Aquifer Water	Empirical	degrees C	7.50	7.50	12.5	12.5	17.5	22.5	22.5	Collins, 1925
AS14	Ambient Groundwater pH	Empirical	standard units	3.20	5.20	6.10	6.83	7.41	7.94	9.68	data from USEPA's STORET database, reported in USEPA, 1997a
AS15	Fraction of Organic Carbon	Johnson SB	unitless	1.67e-05	1.30e-04	2.30e-04	4.33e-04	7.92e-04	1.34e-03	9.04e-03	data from USEPA's STORET database, reported in USEPA, 1997a
AS16	Radial Distance of Well from Downgradient Edge of Waste Unit	Constant	m	150							Policy for Tier 1
AS17	Angle of Well Off Plume Centerline	Constant	degrees	0							Policy for Tier 1
AS20	Depth of Well Below Water Table	Uniform	m	6.19e-05	0.852	2.24	5.49	13.3	35.2	643	API, 1989
AS21	Soil/Water Distribution Coefficient	Derived	cm ³ /g	chemical-specific value							Derived
AS22	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
AS23	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
AS24	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-4. Parameter Values for Waste Piles

Table 2-11 Parameter Values for Waste Piles											
Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Source Parameters											
SS1	Area	Regional Site-Based	m	5.06	20.2	20.2	121	1,380	5,580	2,020,000	USEPA, 1986 and 1997b
SS2	Length	Derived	m	2.25	4.49	4.49	11.0	37.2	74.7	1,420	Derived
SS3	Width	Derived	m	2.25	4.49	4.49	11.0	37.2	74.7	1,420	Derived
SS5	Recharge Rate	Regional Site-Based	m/yr	1.00e-05	5.08e-02	7.87e-02	1.55e-01	3.08e-01	4.38e-01	1.15	ABB, 1995 and USEPA, 1997b
SS6	Infiltration Rate (NO LINER)	Regional Site-Based	m/yr	0.0003	0.0602	0.1283	0.2553	0.3907	0.538	1.264	ABB, 1995 and USEPA, 1997b
SS6	Infiltration Rate (SINGLE LINER)	Regional Site-Based	m/yr	0.00001	0.0297	0.106	0.127	0.133	0.135	0.136	USEPA, 1999
SS6	Infiltration Rate (COMPOSITE LINER)	Regional Site-Based	m/yr	0	0	0	0	7.30e-05	1.78e-04	4.01e-04	TetraTech, 2001
SS10	Operational Life (Leaching Duration)	Constant	yr	20							USEPA, 1996
SS15	Depth of Unit Below Land Surface	Constant	m	0							Assumption of waste pile design
Unsaturated Zone Parameters											
US1	Saturated Hydraulic Conductivity	Based on soil type ²	m/yr	0.00402	0.608	2.13	8.06	34.0	153	2,400	Carsel and Parrish, 1988
US2	Moisture Retention Parameter (alpha)	Based on soil type ²	1/m	0.111	0.618	0.938	1.52	2.69	5.62	20.6	Carsel and Parrish, 1988
US3	Moisture Retention Parameter (beta)	Based on soil type ²	unitless	1.02	1.20	1.26	1.37	1.53	1.81	2.55	Carsel and Parrish, 1988
US4	Residual Water Content	Based on soil type ²	unitless	0.0114	0.0496	0.0613	0.0744	0.0855	0.0935	0.115	Carsel and Parrish, 1988
US5	Saturated Water Content	Based on soil type ²	unitless	0.410	0.410	0.430	0.450	0.450	0.450	0.450	Carsel and Parrish, 1988
US6	Thickness of Unsaturated Zone	Regional Site-Based	m	0.305	1.52	3.66	6.10	15.2	30.5	610	API, 1989
US7	Dispersivity	Derived	m	0.0267	0.0534	0.101	0.154	0.354	0.691	1.00	Gelhar, 1986; EPRI, 1985; USEPA, 1997a
US8	Percent Organic Matter	Based on soil type ²	unitless	0.00229	0.0338	0.0564	0.100	0.178	0.295	3.56	Carsel and others, 1988
US9	Bulk Density	Based on soil type ²	g/cm ³	1.60	1.60	1.65	1.65	1.67	1.67	1.67	Carsel and others, 1988
US10	Soil/Water Distribution Coefficient	Derived	cm ³ /g	chemical-specific value							Derived
US11	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
US12	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
US13	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-4. Parameter Values for Waste Piles

Input No.	Parameter	Input Distribution Type	Units	Percentiles ¹							References
				0	10	25	50	75	90	100	
Saturated Zone Parameters											
AS1	Average Particle Diameter	Empirical	cm	4.00e-04	1.57e-03	5.61e-03	1.92e-02	4.11e-02	7.61e-02	2.12e-01	Shea, 1974
AS2	Aquifer Effective Porosity	Derived	unitless	0.0502	0.106	0.161	0.233	0.296	0.334	0.428	Davis, 1969; McWorter and Sunada, 1977
AS3	Aquifer Bulk Density	Derived	g/cm³	1.16	1.30	1.43	1.56	1.63	1.70	1.80	Freeze and Cherry, 1979
AS4	Aquifer Saturated Thickness	Regional Site-Based	m	0.305	3.05	7.32	12.2	30.5	85.3	914	API, 1989
AS5	Longitudinal Hydraulic Conductivity	Regional Site-Based	m/yr	3.15	63.1	315	1,890	8,650	29,000	7,730,000	API, 1989
AS6	Anisotropy Ratio	Constant	unitless	1							Assumption
AS7	Hydraulic Gradient	Regional Site-Based	unitless	2.00e-06	1.00e-03	2.00e-03	5.70e-03	1.80e-02	3.30e-02	3.42e-01	API, 1989
AS8	Seepage Velocity	Derived	m/yr	0.101	1.94	7.13	38.7	212	1,060	11,000	Derived
AS9	Retardation Factor	Derived	unitless	chemical-specific value							Derived
AS10	Longitudinal Dispersivity	Gelhar Empirical	m	0.101	0.978	3.30	7.15	22.2	72.2	215	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS11	Transverse Dispersivity	Gelhar Empirical	m	0.0126	0.122	0.412	0.894	2.78	9.03	26.9	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS12	Vertical Dispersivity	Gelhar Empirical	m	0.00500	0.00611	0.0206	0.0447	0.139	0.452	1.35	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS13	Temperature of Ambient Aquifer Water	Empirical	degrees C	7.50	7.50	12.5	12.5	17.5	22.5	22.5	Collins, 1925
AS14	Ambient Groundwater pH	Empirical	standard units	3.21	5.11	6.03	6.80	7.40	7.89	9.69	data from USEPA's STORET database, reported in USEPA, 1997a
AS15	Fraction of Organic Carbon	Johnson SB	unitless	1.28e-05	1.30e-04	2.35e-04	4.29e-04	7.98e-04	1.39e-03	1.54e-02	data from USEPA's STORET database, reported in USEPA, 1997a
AS16	Radial Distance of Well from Downgradient Edge of Waste Unit	Constant	m	150							Policy for Tier 1
AS17	Angle of Well Off Plume Centerline	Constant	degrees	0							Policy for Tier 1
AS20	Depth of Well Below Water Table	Uniform	m	3.08e-04	0.850	2.35	5.98	15.8	41.3	892	API, 1989
AS21	Soil/Water Distribution Coefficient	Derived	cm³/g	chemical-specific value							Derived
AS22	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
AS23	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
AS24	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-5. Parameter Values for Land Application Units

Input No.	Parameter	Input Distribution Type	Units	Percentiles ⁶							References
				0	10	25	50	75	90	100	
Source Parameters											
SS1	Area	Regional Site-Based	m	20.2	324	6,070	48,600	243,000	878,000	8.09e+07	USEPA, 1986 and 1997b
SS2	Length	Derived	m	4.49	18.0	77.9	221	493	937	8,990	Derived
SS3	Width	Derived	m	4.49	18.0	77.9	221	493	937	8,990	Derived
SS5	Recharge Rate	Regional Site-Based	m/yr	1.00e-05	2.39e-02	7.98e-02	1.39e-01	2.61e-01	3.53e-01	7.45e-01	ABB, 1995 and USEPA, 1997b
SS6	Infiltration Rate	Regional Site-Based	m/yr	1.00e-05	2.39e-02	7.80e-02	1.21e-01	2.57e-01	3.53e-01	7.45e-01	ABB, 1995 and USEPA, 1997b
SS10	Operational Life (Leaching Duration)	Constant	yr	40							USEPA, 1996
SS15	Depth of Unit Below Land Surface	Constant	m	0							Assumption of LAU design
Unsaturated Zone Parameters											
US1	Saturated Hydraulic Conductivity	Based on soil type ²	m/yr	0.00464	0.613	2.16	8.09	33.6	144	2,400	Carsel and Parrish, 1988
US2	Moisture Retention Parameter (alpha)	Based on soil type ²	1/m	0.0926	0.619	0.945	1.52	2.67	5.81	19.9	Carsel and Parrish, 1988
US3	Moisture Retention Parameter (beta)	Based on soil type ²	unitless	1.02	1.20	1.26	1.37	1.53	1.82	2.55	Carsel and Parrish, 1988
US4	Residual Water Content	Based on soil type ²	unitless	0.0157	0.0494	0.0610	0.0743	0.0858	0.0940	0.115	Carsel and Parrish, 1988
US5	Saturated Water Content	Based on soil type ²	unitless	0.410	0.410	0.430	0.450	0.450	0.450	0.450	Carsel and Parrish, 1988
US6	Thickness of Unsaturated Zone	Regional Site-Based	m	0.305	1.83	3.66	6.10	15.2	36.6	610	API, 1989
US7	Dispersivity	Derived	m	0.0267	0.0603	0.101	0.154	0.354	0.825	1.00	Gelhar, 1986; EPRI, 1985; USEPA, 1997a
US8	Percent Organic Matter	Based on soil type ²	unitless	0.00549	0.0350	0.0584	0.102	0.176	0.293	1.65	Carsel and others, 1988
US9	Bulk Density	Based on soil type ²	g/cm³	1.60	1.65	1.65	1.65	1.65	1.65	1.65	Carsel and others, 1988
US10	Soil/Water Distribution Coefficient	Derived	cm³/g	chemical-specific value							Derived
US11	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
US12	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
US13	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Table 2-5. Parameter Values for Land Application Units

Input No.	Parameter	Input Distribution Type	Units	Percentiles ⁶							References
				0	10	25	50	75	90	100	
Saturated Zone Parameters											
AS1	Average Particle Diameter	Empirical	cm	4.00e-04	1.47e-03	5.35e-03	1.86e-02	4.08e-02	7.82e-02	2.12e-01	Shea, 1974
AS2	Aquifer Effective Porosity	Derived	unitless	0.0501	0.101	0.159	0.233	0.295	0.335	0.429	Davis, 1969; McWorter and Sunada, 1977
AS3	Aquifer Bulk Density	Derived	g/cm³	1.16	1.29	1.43	1.55	1.63	1.70	1.80	Freeze and Cherry, 1979
AS4	Aquifer Saturated Thickness	Regional Site-Based	m	0.305	3.05	6.40	17.9	32.9	91.4	914	API, 1989
AS5	Longitudinal Hydraulic Conductivity	Regional Site-Based	m/yr	3.15	31.5	189	1,580	9,780	27,800	7,190,000	API, 1989
AS6	Anisotropy Ratio	Constant	unitless	1							Assumption
AS7	Hydraulic Gradient	Regional Site-Based	unitless	2.00e-06	6.71e-04	2.00e-03	8.51e-03	2.30e-02	4.30e-02	2.71e-01	API, 1989
AS8	Seepage Velocity	Derived	m/yr	0.100	1.46	5.89	30.0	201	919	10,400	Derived
AS9	Retardation Factor	Derived	unitless	chemical-specific value							Derived
AS10	Longitudinal Dispersivity	Gelhar Empirical	m	0.108	1.44	4.47	9.43	33.2	92.9	324	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS11	Transverse Dispersivity	Gelhar Empirical	m	0.0134	0.180	0.558	1.18	4.15	11.6	40.5	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS12	Vertical Dispersivity	Gelhar Empirical	m	0.00500	0.00901	0.0279	0.0590	0.207	0.580	2.03	EPRI, 1985; Gelhar, 1986; Gelhar, 1992
AS13	Temperature of Ambient Aquifer Water	Empirical	degrees C	7.50	7.50	12.5	12.5	17.5	17.5	22.5	Collins, 1925
AS14	Ambient Groundwater pH	Empirical	standard units	3.21	5.19	6.05	6.82	7.39	7.88	9.69	data from USEPA's STORET database, reported in USEPA, 1997a
AS15	Fraction of Organic Carbon	Johnson SB	unitless	1.21e-05	1.29e-04	2.28e-04	4.27e-04	7.85e-04	1.34e-03	1.20e-02	data from USEPA's STORET database, reported in USEPA, 1997a
AS16	Radial Distance of Well from Downgradient Edge of Waste Unit	Constant	m	150							Policy for Tier 1
AS17	Angle of Well Off Plume Centerline	Constant	degrees	0							Policy for Tier 1
AS20	Depth of Well Below Water Table	Uniform	m	9.63e-05	0.886	2.38	6.63	17.4	47.2	882	API, 1989
AS21	Soil/Water Distribution Coefficient	Derived	cm³/g	chemical-specific value							Derived
AS22	Freundlich Adsorption Isotherm Exponent	Constant	unitless	1							Assumption
AS23	Hydrolysis Degradation Rate Coefficient	Derived	1/yr	chemical-specific value							Derived
AS24	Biodegradation Rate Coefficient	Constant	1/yr	0							Policy for Tier 1

Footnotes for Tables 2-2, 2-3, 2-4, and 2-5

¹ Values were generated using a Monte Carlo simulation with 10,000 iterations.

² The actual distribution type depends upon the soil type. Since the soil type is automatically varied in a site-based Monte Carlo run, the distribution of values shown here are the net result based on data for all three soil types. The distribution type for each soil parameter per soil type is given in the table below.

Parameter	Soil Type		
	Sandy Clay Loam	Silt Loam	Sandy Loam
Saturated Hydraulic Conductivity	Johnson SB (log ratio)	Lognormal	Johnson SB (log ratio)
Moisture Retention Parameter (alpha)	Johnson SB (log ratio)	Lognormal	Johnson SB (log ratio)
Moisture Retention Parameter (beta)	Normal	Johnson SB (log ratio)	Lognormal
Residual Water Content	Normal	Johnson SB (log ratio)	Johnson SB (log ratio)
Saturated Water Content	Constant	Constant	Constant
Percent Organic Matter	Johnson SB (log ratio)	Johnson SB (log ratio)	Johnson SB (log ratio)
Bulk Density	Constant	Constant	Constant

³ While these input values cannot be specified by the user in the input file (they are either internally set to a constant value or derived automatically by the EPACMTP model), these data are presented here because they are important in determining the model output.

⁴ These values are not standard output and were therefore computed in a spreadsheet using the EPACMTP values generated for this scenario.

⁵ These values are not standard output and were therefore computed by hand using a series of random numbers and the EPACMTP values generated for this scenario.

⁶ Values were generated using a Monte Carlo simulation with 6,557 iterations.

2.3 References for Section 2.0

- ABB Environmental Services. 1995. Estimation of Leachate Rates from Industrial Waste Management Facilities. August, 1995.
- API. 1989. Hydrogeologic Database for Groundwater Modeling. API Publication No. 4476, American Petroleum Institute.
- Bonaparte, R., J.P. Giroud, and B.A. Gross. 1989. Rates of leakage through landfill liners. Geosynthetics 1989 Conference, San Diego, California.
- Carsel, R.F., and R.S. Parrish. 1988. Developing joint probability distributions of soil water retention characteristics. *Water Resources Research* 29:755-770.
- Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. Characterizing the uncertainty of pesticide leaching in agricultural soils. *Journal of Contaminant Hydrology*, 2: 111-124.
- Collins, W.D. 1925. Temperature of water available for industrial use in the United States. US Geological Survey Water-Supply Paper 520-F, pp.97-104.
- Davis, S.N. 1969. Porosity and permeability of natural materials. In: *Flow Through Porous Media*, R.J.M. de Wiest, Editor, Academic Press, NY.
- Eith, A.W. and G.R. Koerner. 1997. Assessment of HDPE geomembrane performance in a municipal waste landfill double liner system after eight years of service. *Geotextiles and Geomembranes*, vol. 15, pp. 277-287.
- Electric Power Research Institute (EPRI). 1985. A review of Field Scale Physical Solute Transport Processes in Saturated and Unsaturated Porous Media. EPRI EA-4190, Project 2485-5, Palo Alto, California.
- Freeze, R.A. and J. Cherry. 1979. *Groundwater*. Prentice-Hall, Englewood Cliffs, NJ.
- Gelhar, L.W. 1986. Personal Communication with Zubair Saleem.
- Gelhar, L.W., C. Welty, K.R. Rehfeldt. 1992. A critical review of data on field-scale dispersion in aquifers. *Water Resource Research*, 28(7), 1955-1974.

- Giroud, J.P. and R. Bonaparte. 1989. Leakage through Liners Constructed with Geomembranes – Part I. Geomembrane Liners. *Geotextiles and Geomembranes*, vol 8, pp 27-67.
- Laine, D.L. 1991. Analysis of pinhole seam leaks located in geomembrane liners using the electrical leak location method: Case histories. *Proceedings, Geosynthetics '91*, IFAI, Atlanta, pp. 239-253.
- McQuade, S.J. and A.D. Needham. 1999. Geomembrane liner defects-causes, frequency, and avoidance. *Proceedings of the Institution of Civil Engineers, Geotechnical Engineering*, vol. 137, no. 4, pp. 203-213.
- McWorter, D.B. and D.K. Sunada. 1977. *Groundwater and Hydraulics*, Water Resources Publications, Fort Collins, CO.
- Rollin, A.L., M. Marcotte, T. Jacquelin, and L. Chaput. 1999. Leak location in exposed geomembrane liners using an electrical leak detection technique. *Geosynthetics '99 Specifying Geosynthetics and Developing Design Details*, vol. 2, pp. 615-626.
- Schanz, R. and A. Salhotra. 1992. Subtitle D Landfill Characteristics. Center for Modeling and Risk Assessment, Woodward-Clyde Consultants, Oakland, CA.
- Shea, J.H. 1974. Deficiencies of clastic particles of certain sizes. *Journal of Sedimentary Petrology*, 44(4):985-1003, December.
- Tedder, R.B. 1997. Evaluating the performance of Florida double-lined landfills. *Geosynthetics '97 Conference Proceedings*, IFAI, St. Paul, Minnesota, pp. 425-438.
- Tetra Tech, Inc. 2001. Characterization of Infiltration Rate Data to Support Groundwater Modeling Efforts (Draft). Prepared for the U.S. Environmental Protection Agency, Office of Solid Waste, Contract #68-W6-0061. May, 2001.
- USEPA. 1986. Industrial Subtitle D Facility Study (Telephone Survey), USEPA, October 20, 1986. Washington, DC, 20460.
- USEPA. 1996. EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) Background Document. USEPA Office of Solid Waste, Washington, DC, 20460.
- USEPA. 1997a. EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) Users Guide. USEPA Office of Solid Waste, Washington, DC, 20460.

USEPA. 1997b. Analysis of EPA's Industrial Subtitle D Databases used in Groundwater Pathway Analysis of the Hazardous Waste Identification Rule (HWIR). Office of Solid Waste, Washington, DC.

USEPA. 1998. Assessment and Recommendations for Optimal Performance of Waste Containment Systems. Office of Research and Development, National Risk Management Research Laboratory, Cincinnati, Ohio. Draft Final.

USEPA. 1999. Technical Background Document: Industrial Waste Management Evaluation Model (IWEM), Groundwater Model to Support the Guide for Industrial Waste Management, Draft. USEPA 530-R-99-002.

USEPA. 2001. Industrial Surface Impoundments in the United States. USEPA Office of Solid Waste, Washington, DC, 20460. USEPA 530-R-01-005.

3.0 MCLs AND HEALTH-BASED NUMBERS

The Tier 1 tool incorporates two “Toxicity Reference Levels” (TRLs):

Maximum Contaminant Levels (MCLs). MCLs are available for some of the Tier 1 contaminants. MCLs are maximum permissible contaminant concentrations allowed in public drinking water and are established under the Safe Drinking Water Act. In developing MCLs, EPA considers not only a contaminant’s health effects, but also additional factors, such as the cost of treatment.

Health-based numbers (HBNs). HBNs are available for all of the Tier 1 contaminants. To calculate HBNs, we only consider parameters that describe a contaminant’s toxicity and an individual’s (receptor’s) exposure to the contaminant. For the purposes of developing the Tier 1 tool, HBNs are the maximum contaminant concentrations in groundwater that we expect will not usually cause adverse noncancer health effects in the general population (including sensitive subgroups), or that will not result in an additional incidence of cancer in more than approximately one in one million individuals exposed to the contaminant. Lower concentrations of the contaminant are not likely to cause adverse health effects, except, for example, in individuals exposed to multiple contaminants that produce the same health effect. Similarly, we might expect to find a higher incidence of cancer among sensitive subgroups, highly exposed subpopulations, or populations exposed to more than one cancer-causing contaminant.

The MCLs and the HBNs in the revised Tier 1 tool will differ from those in the draft (1999) Tier 1 tool in the following respects:

- We expanded the HBNs to include not only HBNs that are based on ingestion exposures, but also HBNs that are based on inhalation exposures. An “inhalation HBN” is the maximum concentration of a contaminant in groundwater that is not expected to cause adverse noncancer health effects in most adults, or no more than one additional cancer in one million adults, who inhale the contaminant as a result of activities associated with showering.
- The draft HBNs were those used in EPA’s 1995 Hazardous Waste Identification Rule (HWIR95; 60 Federal Register 66344). These HBNs were calculated using only exposure factors for adults. Consistent with current EPA policy (see Executive Order 13045, <http://www.epa.gov/children/whatwe/executiv.htm>), we revised the ingestion HBNs so that they now reflect consideration of children’s exposure.
- In some cases, the human health benchmarks that served as the basis of the HWIR95 HBNs are outdated. In calculating revised HBNs, we made sure to use the most recently available

human health benchmarks. Attachment C provides the human health benchmarks that we used to calculate the HBNs for the revised Tier 1 tool.

- We recompiled the list of MCLs to ensure that we use only the most recent MCLs in developing the revised Tier 1 tool. (The MCLs in the draft tool were current as of 1996.)

The sections below provide our methodology for calculating the cancer and noncancer HBNs for ingestion and inhalation of the contaminants included in the Tier 1 tool. We calculated the revised HBNs by “rearranging” standard risk equations (see EPA’s *Risk Assessment Guidance for Superfund: Volume 1 – Human Health Evaluation Manual* [USEPA, 1991]) so that we could calculate contaminant concentration, rather than cancer risk or noncancer hazard. The standard equations for cancer risk and noncancer hazard are comprised of two sets of variables: variables that describe an individual’s exposure to a contaminant and a variable that describes the toxicity of the contaminant.

Exposure is the condition that occurs when a contaminant comes into contact with the outer boundary of the body, such as the mouth and nostrils. Once EPA establishes the concentrations of contaminants at the points of exposure, we can estimate the magnitude of each individual’s exposure, or the dose of contaminant. The dose is the amount of the contaminant that crosses the outer boundary of the body and is available for absorption at internal exchange boundaries (lungs, gut, skin) (USEPA, 1992). For example, given an exposure to a carcinogen through ingestion of contaminated drinking water, dose is a function of the concentration of the contaminant in drinking water (assumed to be the concentration of the contaminant at the receptor well), as well as certain “exposure factors,” such as how much drinking water the individual consumes each day (the intake rate), the period of time over which the individual is exposed to the contaminated drinking water (the exposure duration), how often the individual is exposed to contaminated drinking water during the exposure duration (the exposure frequency), and the body weight of the individual. For effects such as cancer, where we usually describe the biological response in terms of lifetime probabilities even though exposure does not occur over the entire lifetime, we average doses over an individual’s lifetime, which we call the “averaging time.”

Contaminant toxicity is described through the use of “human health benchmarks.” Human health benchmarks are quantitative expressions of dose-response relationships. Human health benchmarks include:

- Oral cancer slope factors (CSFo) for oral exposure to carcinogenic (cancer-causing) contaminants;
- Reference doses (RfD) for oral exposure to contaminants that cause noncancer health effects;
- Inhalation cancer slope factors (CSFi), that are derived from Unit Risk Factors (URFs), for inhalation exposure to carcinogenic contaminants; and

- Reference concentrations (RfC) for inhalation exposure to contaminants that cause noncancer health effects.

EPA defines the cancer slope factor (CSF) as: “an upper bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime exposure to an agent [contaminant].” Because the CSF is an upper bound estimate of increased risk, EPA is reasonably confident that the “true risk” will not exceed the risk estimate derived using the CSF and that the “true risk” is likely to be less than predicted. CSFs are expressed in units of proportion (of a population) affected per milligram/kilogram/day (mg/kg/day). For non-cancer health effects, we use the RfD and the RfC as health benchmarks for ingestion and inhalation exposures, respectively. RfDs and RfCs are estimates of daily oral exposure (in the case of an RfD) or a continuous inhalation exposure (in the case of an RfC) that is likely to be without an appreciable risk of adverse effects in the general population, including sensitive individuals, over a lifetime. The methodology used to develop RfDs and RfCs is expected to have an uncertainty spanning an order of magnitude.

We combine estimates of contaminant dose and estimates of contaminant toxicity (the health benchmarks) to calculate estimates of excess lifetime cancer risk for individuals who may be exposed to carcinogenic contaminants and hazard quotients (HQs) for those contaminants that produce noncancer health effects. Excess lifetime cancer risk is the incremental probability (chance) of an individual developing cancer over a lifetime as a result of exposure to a carcinogen. We estimate cancer risk resulting from exposure to a carcinogenic contaminant by multiplying the contaminant’s CSF by our estimate of contaminant dose. We calculate a receptor’s ingestion hazard quotient resulting from exposure to a noncarcinogenic contaminant by dividing our estimate of daily contaminant dose by the RfD (the hazard quotient is the ratio of an individual’s chronic daily contaminant dose to the RfD for chronic exposures to the contaminant). We calculate a receptor’s inhalation hazard quotient by dividing the concentration of the contaminant in air by the RfC.

We developed the Tier 1 HBNs to correspond to a “target risk” and a “target hazard quotient.” The target risk we use to calculate the HBNs for carcinogens is 1×10^{-6} (one in one million). The target hazard quotient we use to calculate the HBNs for noncarcinogens is 1 (unitless). A hazard quotient of 1 indicates that the estimated dose is equal to the RfD and, therefore, an HQ of 1 is frequently EPA’s threshold of concern for noncancer effects. These targets are used to calculate separate HBNs for each contaminant of concern, and separate HBNs for each exposure route of concern (ingestion or inhalation). The Tier 1 tool does not consider combined exposure from groundwater ingestion (from drinking water) and groundwater inhalation (from showering), nor does the Tier 1 tool consider the potential for additive exposure to multiple contaminants.

Usually, doses less than the RfD (HQ=1) are not likely to be associated with adverse health effects and, therefore, are less likely to be of regulatory concern. As the frequency and/or magnitude of

the exposures exceeding the RfD increase (HQ>1), the probability of adverse effects in a human population increases. However, it should not be categorically concluded that all doses below the RfD are “acceptable” (or will be risk-free) and that all doses in excess of the RfD are “unacceptable” (or will result in adverse effects). Table 3-5, presented at the end of Section 3, provides the revised MCLs and HBNs we are using to develop the Tier 1 tool.

3.1 Ingestion HBNs

Section 3.1.1 describes how we calculated ingestion HBNs for contaminants that cause cancer, and Section 3.1.2 describes how we calculated ingestion HBNs for contaminants that cause adverse health effects other than cancer.

3.1.1 Ingestion HBNs for Contaminants That Cause Cancer

To calculate ingestion HBNs for carcinogens, we rearranged the standard equation for estimating risk so that instead of solving for risk, we solve for contaminant concentration in water. The contaminant concentration in water that corresponds to the target cancer risk is the cancer HBN for ingestion exposures, as follows:

$$C_INGEST_HBN = \frac{Risk_target \cdot AT \cdot 365}{CSFo \cdot EF \cdot ED \cdot CRw}$$

where

C_INGEST_HBN	=	cancer HBN for ingestion of water (mg/L)
Risk_target	=	target risk for carcinogens = 1×10^{-6}
CSFo	=	contaminant -specific oral cancer slope factor (mg/kg-d) ⁻¹
AT	=	averaging time = 70 years [yrs]
EF	=	exposure frequency = 350 d/yr
CRw	=	intake rate of water = 0.0252 L/kg/d
ED	=	exposure duration = 30 yr
365	=	conversion factor (d/yr).

In this equation, the CSFo quantifies the toxicity of the contaminant. The averaging time, exposure frequency, intake rate of water (which is expressed as the amount of water an individual consumes each day per kilogram of their body weight), and exposure duration quantify aspects of an individual's exposure. In our calculation of cancer and noncancer ingestion HBNs, we use data that combine the factors for intake rate and body weight. That is, we express intake in terms of the amount of water an individual consumes per kilogram (kg) of their body weight. For example, if an individual consumes 2 liters (L) of water per day (d), and that individual weighs 65 kg, then their intake would be

2 L/d per 65 kg, or 0.03 L/kg/d. Table 3-1 summarizes the basis for the exposure parameter values that we used in this equation.

Table 3-1. Exposure Parameter Values for Ingestion HBNs – Carcinogens

Exposure Parameter	Value	Units	Source
Drinking Water Intake Rate	25.2	mL/kg/d	The value is a time-weighted average of mean drinking water intake rates (per kilogram body weight) for individuals aged 0 to 29 years. Table 3-7 of the <i>Exposure Factors Handbook</i> (USEPA, 1997a)
Exposure Frequency	350	d/yr	The exposure frequency is the number of days per year that an individual is exposed. A value of 350 days per year considers that an individual is away from home for 2 weeks per year. <i>Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual</i> (US EPA, 1991)
Exposure Duration	30	yr	The exposure duration is the number of years that an individual is exposed. Thirty years is the 95 th percentile value for population mobility (exposure duration). Table 15-176 of the <i>Exposure Factors Handbook</i> (USEPA, 1997b)
Averaging Time	70	yr	Averaging time is the period of time over which a receptor's dose is averaged. When evaluating carcinogens, dose is averaged over the lifetime of the individual, assumed to be 70 years. <i>Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual</i> (US EPA, 1991)

3.1.2 Ingestion HBNs for Contaminants that Cause Noncancer Health Effects

To calculate ingestion HBNs for contaminants that cause health effects other than cancer, we rearranged the standard equation for estimating hazard quotient so that instead of solving for the hazard quotient, we solve for contaminant concentration in water. The contaminant concentration in water that corresponds to the target hazard quotient is the cancer HBN for ingestion exposures, as follows:

$$NC_INGEST_HBN = \frac{HQ_target \cdot RfD \cdot 365}{EF \cdot CRw}$$

where

NC_INGEST_HBN	=	noncancer HBN for ingestion of water (mg/L)
HQ_target	=	target hazard quotient for noncarcinogens = 1
RfD	=	contaminant-specific reference dose (mg/kg-d)
EF	=	exposure frequency = 350 d/yr
CRw	=	intake rate of water = 0.0426 L/kg/d
365	=	conversion factor (d/yr).

In this equation, the exposure frequency and intake rate of water (expressed as the amount of water an individual consumes each day per kilogram of body weight) quantify aspects of an individual's exposure. To develop noncancer ingestion HBNs that are protective of children, the intake rate in this equation assumes that the individual who is drinking water from the modeled receptor well is a child who is exposed from age 0 to 6 years. Children in this age range typically ingest greater amounts of water per unit body weight (have greater exposure) than do adults.

The RfD in the equation quantifies the toxicity of the contaminant. Even though the RfDs that we use in this analysis are defined to pertain to exposures that occur over a lifetime, these "chronic" RfDs commonly are used to evaluate potential noncancer effects associated with exposures that occur over a significant portion of a lifetime (generally assumed to be between seven years and a lifetime). We do not average the dose for noncarcinogens over the lifetime of an individual (the "averaging time") as we do for carcinogens, rather, we average dose over only the period of exposure. Consequently, the values for exposure duration and averaging time are the same, and cancel each other out (that is why they are not included in the above equation). Table 3-2 summarizes the basis for the exposure parameter values that we used in this equation.

Table 3-2. Exposure Parameter Values for Ingestion HBNs – Noncarcinogens

Exposure Parameter	Value	Units	Source
Drinking Water Intake Rate	42.6	mL/kg/d	The value is a time-weighted average of mean drinking water intake rates (per kilogram body weight) for children aged 0 to 6 years. Table 3-7 of the <i>Exposure Factors Handbook</i> (USEPA, 1997a)
Exposure Frequency	350	d/yr	The exposure frequency is the number of days per year that an individual is exposed. A value of 350 days per year considers that an individual is away from home for 2 weeks per year. <i>Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual</i> (US EPA, 1991)

3.2 Inhalation HBNs

In the Tier 1 tool, the inhalation HBN is the maximum concentration of a contaminant in groundwater that is not expected to cause adverse health effects in most adults who inhale the contaminant as a result of activities associated with showering. We did not evaluate children's shower-related exposure in developing inhalation HBNs because we assume that children take baths. Because we have not yet developed a "bath model" for evaluating children, we do not have inhalation HBNs that consider children's exposure. We calculated inhalation HBNs only for contaminants that (1) volatilize (that is, mercury and organic contaminants) and (2) have an inhalation health benchmark available (that is, a reference concentration [RfC], inhalation unit risk factor [URF], and/or inhalation cancer slope factor [CSFi]).

We developed the inhalation HBNs as follows:

First, we used a shower model to calculate, on a per unit groundwater concentration basis, the average concentration of each contaminant in indoor air that an adult will be exposed to daily as a result of activities associated with showering. In this analysis, we assume that the shower water is groundwater from the receptor well modeled in the Tier 1 analysis (the contaminant concentration in groundwater at the receptor well). However, in this step of the analysis we only have to model a "unit" groundwater concentration. This is because the average concentration of a contaminant in indoor air is directly proportional to the concentration of the contaminant in the water coming into the shower. As a result, we can back-calculate the groundwater concentration that would result in any given contaminant concentration in indoor air by simple scaling. Section 3.2.1 describes how we use the shower model to calculate the average concentration of a contaminant in indoor air to which an adult is exposed during the day.

Second, we used the unit average contaminant concentration in indoor air, determined above, to calculate the HBN. We first calculated the risk or hazard quotient associated with the unit air concentration from the shower model, and then scaled this result to determine the groundwater concentration associated with the target risk level or target hazard quotient. The groundwater concentration that generates the air concentration associated with a risk of 1×10^{-6} or a hazard quotient of 1 is the inhalation HBN. Section 3.2.2 describes how we calculated inhalation HBNs for cancer-causing chemicals and for chemicals that cause non-cancer health effects.

3.2.1 Calculation of Exposure Concentrations from Showering

Individuals may be exposed to contaminants through inhalation of air-phase emissions from groundwater. Such exposure may occur during the time spent in the shower while showering, in the shower stall after showering, and in the bathroom after showering. To evaluate these exposures, EPA uses a shower model to estimate contaminant concentrations in a shower stall and in bathroom air. This section describes the shower model (Section 3.2.1.1) and the uncertainties and limitations associated with its use (Section 3.2.1.2).

A primary assumption of our evaluation is that contaminants are released into household air only as the result of showering activity, and that exposure to air-phase contaminants only occurs in the shower stall and in the bathroom. Some investigators evaluate contaminant emissions resulting from other household uses of water (for example, use of water in sinks, toilets, washing machines, and dishwashers) and the associated inhalation exposure that occurs during the time spent in the non-bathroom portions of the house ("the remainder of the house"). The model described below only focuses on exposure in the shower stall and bathroom, and the exposure that results from showering. Section 3.2.1.2 discusses this limitation of the model in greater detail.

3.2.1.1 Shower Model

The shower model calculates the incremental change in the concentration of a contaminant in air that results from the transfer of contaminant 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 contaminant 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 contaminant concentration in the shower stall and bathroom, we use those concentrations to estimate the average air-phase contaminant concentration to which an individual is exposed over the course of an entire day. We use this average daily concentration to calculate an inhalation HBN, as described in Section 3.2.2.

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 A-1 to A-11 in Attachment A. In reviewing the equations and reading the following sections, it will help to keep in mind the following two concepts:

We calculate air-phase contaminant 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 A-1 and A-2).

We calculate air-phase contaminant concentrations for different time steps. We implement the shower model in time steps. That is, we estimate the air-phase contaminant concentration in each of the two compartments in 0.2-minute increments or time steps. The air-phase contaminant 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 contaminant mass from the shower water (which adds contaminant 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 contaminant;
- Estimate the air-phase contaminant concentration in the shower stall for sequential 0.2-minute time steps;
- Estimate the air-phase contaminant concentration in the bathroom (other than in the shower stall) for sequential 0.2-minute time steps;
- Use the air-phase contaminant concentrations calculated for the shower stall, and the air-phase contaminant concentrations calculated for the bathroom, to calculate the average contaminant concentration to which an adult is exposed during the course of a day.

This procedure is explained in greater detail below. Attachment B provides the values for the contaminant-specific properties used in the model. Table 3-3 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 contaminant in air is to quantify the contaminant's "resistance" to movement between the water phase and the air phase. We quantify this resistance using the mass transfer coefficient presented in Equation A-4, which incorporates variables calculated in Equations A-3 and A-5. The mass transfer coefficient depends on properties specific to each contaminant evaluated, as well as physical properties of the water droplet. Specifically, the mass transfer coefficient depends on:

- The contaminant's diffusivity in water (the molecular diffusion coefficient for the contaminant in water), which determines how readily the contaminant mass in the center of the water droplet will diffuse to the surface of the water droplet. If a contaminant's diffusivity in water is low, then as the contaminant is emitted from the surface of the water droplet, the rate at which the surface of the droplet is "supplied" with contaminant from the center of the water droplet will be slow, resulting in less contaminant being emitted from the droplet. Diffusivity influences the concentration gradient across the droplet.
- The Henry's law constant for the contaminant, which establishes how the contaminant will partition between the water phase and the air phase to achieve equilibrium. Henry's law states that, at equilibrium, the amount of a contaminant dissolved in water is proportional to the amount of the contaminant in the air phase that is in contact with the water. This proportion is contaminant-specific (each contaminant has a different Henry's law constant). The Henry's law constant influences the magnitude of the air-phase contaminant concentrations more than any other contaminant-specific parameter.
- The contaminant's diffusivity in air (the molecular diffusion coefficient for the contaminant in air), which determines how readily the contaminant will migrate away from the droplet once it is released into the air surrounding the droplet. Contaminants 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 contaminant 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 3-3.

Table 3-3. 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	USEPA, 1997c	Table 15-23. 50th percentile overall
T_bathroom	Time spent in bathroom, not in shower	5	min	USEPA, 1997c	Table 15-32. 50th percentile overall
ShowerTime	Shower time, 50th percentile	15	min	USEPA, 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 ≤ 600 cm/sec (Coburn, 1996).
Groundwater					
Cin	Contaminant concentration in incoming water	0.001	mg/L	NA	Unit concentration selected.

- 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 3-3).

Attachments B presents the contaminant-specific diffusivities and Henry's law constants that we used in our analysis.

Calculating the Air-Phase Contaminant Concentration in the Shower

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

1. Calculating the fraction of contaminant that can be emitted into the air from each water droplet (Equation A-7);
2. Translating the fraction of contaminant that can be emitted from each water droplet (from step 1) into the mass of contaminant that is emitted from the entire volume of water that is coming into the shower during each time step (Equation A-6); and
3. Determining the contaminant concentration at the end of the time step by: calculating the concentration added to the shower air during the time step (dividing the contaminant mass emitted from the water in step 2 by the volume of the shower), adding this concentration to the concentration of the contaminant 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 A-9).

An important element of this analysis is the difference between the time in the shower stall that is spent showering (15 minutes, Table 3-3) and the time in the shower stall that occurs after showering (5 minutes, Table 3-3). The difference in these two time periods involves how we handle the value for mass of contaminant 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 contaminant is only a function of the concentration of the contaminant 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 contaminant mass that potentially can be emitted from a droplet at any given time during the droplet's fall through the air (Equation A-7) is a function of the mass transfer coefficient (the contaminant'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 A-8). Inherent in this calculation is an assumption that the concentration of the contaminant 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 contaminant concentration is to the maximum possible (equilibrium) air-phase concentration. Stated another way, Henry's law dictates that for a certain contaminant concentration in water, we can predict the maximum concentration of contaminant in the air that is in contact with the water (assuming the air and water are in equilibrium). Consequently, if there is already contaminant in the air, then, to maintain equilibrium, there is a limit to how much additional contaminant can be emitted from the water to the air (the less contaminant already present in the air, the more contaminant 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 contaminant will "free itself" from the water. Factor's such as the contaminant's dispersivity (in water and air) and the surface area of the droplet also influence the fraction of contaminant mass that can be emitted from the droplet.

In most cases, for each 0.2-minute time step we evaluate, the mass of a contaminant emitted from the shower water to the air is the product of: the concentration of the contaminant in the shower water, the volume of water emitted from the shower during the time step, and the fraction of the contaminant 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 contaminant mass that can be emitted from the shower water during the time step. The cap is the maximum contaminant mass that could be emitted from the water at equilibrium (based on Henry's law) minus the contaminant mass already in the shower stall at the beginning of the time step

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

The air-phase contaminant concentration in the bathroom (Equation A-10) is a function of the air-phase contaminant 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 contaminant concentration in the bathroom is equal to: the air-phase contaminant concentration in the bathroom at the beginning of the time step, plus the contaminant concentration added as a result of the exchange of air with the shower, minus the contaminant

concentration lost as a result of the exchange of air with the rest of the house. Table 3-3 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 Contaminant Concentration to Which an Individual is Exposed

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

1. Calculate the average contaminant 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 A-2);
2. Calculate the average contaminant 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 contaminant in the shower, and in the bathroom after showering (that is, that the concentration of the contaminant in the rest of the house is zero).

3.2.1.2 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 contaminant 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 expected the lower risk due to exposure in the remainder of the house, and the lack of available data to estimate house

contaminant 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" (USEPA, 2000).
- Our analysis does not consider either 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 contaminant concentrations.
- A contaminant'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 contaminant in water exceeds the contaminant's solubility in that water, we expect that at least some of the contaminant will exist in the water as a non-aqueous (free)

phase. Henry's law, a basic principle of the shower model, only applies to contaminants dissolved in water, it does not apply to non-aqueous phase contaminants (USEPA, 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 groundwater well) contained non-aqueous phase contaminant. More importantly, however, EPACMTP, the groundwater fate and transport model that we use to estimate contaminant concentrations in the modeled groundwater, cannot be used to model non-aqueous phase liquids. Consequently, the Tier 1 tool should not be used in cases where non-aqueous phase contaminants are present in leachate. In these situations, another tool must be used that is capable of evaluating non-aqueous phase liquids.

3.2.2 Calculating Inhalation HBNs

To calculate HBNs, we selected a unit groundwater concentration (usually 1 mg/L) within the solubility limits of each contaminant and implemented the shower model using that concentration. The result of the shower model was the average concentration of a contaminant in air to which an individual is exposed on a daily basis. We used this "unit" air concentration to calculate a corresponding "unit" risk (for cancer-causing chemicals) or "unit" hazard quotient (for contaminants that cause noncancer health effects). Because groundwater concentration and inhalation risk or hazard are directly proportional, we used simple ratios to adjust the unit groundwater concentration to the groundwater concentration corresponding to the target risk or target hazard quotient (that is, to calculate the inhalation HBNs). Section 3.2.2.1 describes our application of this methodology to carcinogens and Section 3.2.2.2 describes our application of this methodology to noncarcinogens.

3.2.2.1 Inhalation HBNs for Carcinogens

Using the shower model, we estimated the average concentration of a contaminant in air to which an individual is exposed on a daily basis. To calculate the inhalation HBN for carcinogens, we first calculate the inhalation risk that corresponds to this modeled contaminant concentration:

$$Risk_{modeled} = \frac{(Cair_{modeled} \cdot IR \cdot ED \cdot EF)}{(BW \cdot AT \cdot 365)} \cdot CSFi$$

where

Risk_modeled	=	inhalation risk resulting from the modeled contaminant concentration in air
Cair_modeled =		average contaminant concentration in air to which an individual is exposed during a day (mg/m ³) (calculated from the unit groundwater concentration using the shower model)
IR	=	inhalation rate = 13.25 m ³ /d
ED	=	exposure duration = 30 yr
EF	=	exposure frequency = 350 d/yr
BW	=	body weight (kg) = 71.8 kg
AT	=	averaging time = 70 yr
CSFi	=	contaminant-specific inhalation cancer slope factor (mg/kg-d) ⁻¹
365	=	conversion factor (d/yr).

In this equation, the CSFi quantifies the toxicity of the contaminant. We use the average contaminant concentration in air, inhalation rate, exposure duration, exposure frequency, body weight, and averaging time to quantify the individual's exposure, or dose. Table 3-4 summarizes the basis for the exposure parameter values used in this equation.

Table 3-4. Exposure Parameter Values for Inhalation HBNs

Exposure Parameter	Value	Units	Source
Inhalation Rate	13.25	m ³ /d	The value corresponds to the mean inhalation rates for adults (ages 19 to 65+). The value was calculated by averaging the daily mean inhalation rates for females (11.3 m ³ /d) and males (15.2 m ³ /d).
Body Weight	71.8	kg	Table 5-23 of the <i>Exposure Factors Handbook</i> (USEPA, 1997a)
Exposure Frequency	350	d/yr	The value corresponds to the mean body weight of 18- to 75-year-old men and women. Tables 7-2 and 7-11 of the <i>Exposure Factors Handbook</i> (USEPA, 1997a)
Exposure Duration	30	yr	The exposure frequency is the number of days per year that an individual is exposed. A value of 350 days per year considers that an individual is away from home for 2 weeks per year. <i>Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual</i> (U.S. EPA, 1991)
Averaging Time	70	yr	The exposure duration is the number of years that an individual is exposed. Thirty years is the 95 th percentile value for population mobility (exposure duration). Table 15-176 of the <i>Exposure Factors Handbook</i> (USEPA, 1997b)
			<i>Risk Assessment Guidance for Superfund: Volume 1—Human Health Evaluation Manual</i> (U.S. EPA, 1991)

The modeled contaminant concentration in air was based on evaluating a unit contaminant concentration in groundwater (a contaminant concentration in groundwater that we selected somewhat arbitrarily). To calculate the groundwater concentration that corresponds to the target inhalation risk (that is, the inhalation HBN) we adjusted the modeled unit groundwater concentration using a simple ratio of target risk and modeled risk:

$$C_INHALE_HBN = \frac{Risk_target}{Risk_modeled} \cdot C_GW_modeled$$

where

C_INHALE_HBN	=	concentration in groundwater resulting in target risk (µg/L) (cancer HBN for inhalation)
C_GW_modeled	=	unit concentration in groundwater used in shower model (µg/L)
Risk_target	=	target risk for carcinogens = 1 x 10 ⁻⁶
Risk_modeled	=	risk resulting from groundwater concentration modeled.

This equation assumes that groundwater concentration and inhalation risk are directly proportional, which we confirmed by running the shower model using the target groundwater concentration (the inhalation HBN) for several contaminants and comparing the results to the target risk level.

3.2.2.2 Inhalation HBNs for Noncarcinogens

Calculating inhalation HBNs for noncarcinogens is simpler than calculating HBNs for carcinogens because the toxicity benchmark (RfC) is expressed as a concentration in air. To calculate the HBN, we first determine the hazard quotient resulting from the unit air concentration output by the shower model:

$$HQ_modeled = \frac{Cair_modeled}{RfC}$$

where

HQ_modeled	=	hazard quotient resulting from the groundwater concentration modeled (unitless)
Cair_modeled	=	average air concentration to which an individual is exposed during a day (mg/m ³) (calculated from the unit groundwater concentration using the shower model)
RfC	=	contaminant-specific reference concentration (mg/m ³).

We then derive the target groundwater concentration (that is, the inhalation HBN) by adjusting the modeled unit groundwater concentration using the ratio of the target hazard quotient to the modeled hazard quotient:

$$NC_INHALE_HBN = \frac{HQ_target}{HQ_modeled} \cdot C_GW_modeled$$

where

NC_INHALE_HBN	=	concentration in groundwater resulting in target hazard quotient (µg/L) (noncancer HBN for inhalation)
C_GW_modeled	=	unit concentration in groundwater used in shower model (µg/L)
HQ_target	=	target hazard quotient for noncarcinogens = 1
HQ_modeled	=	hazard quotient resulting from groundwater concentration modeled.

Table 3-5. Tier 1 MCLs and HBNs

CAS Number	Chemical Name	MCL (mg/L)	Ingestion HBNs		Inhalation HBNs	
			Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)	Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)
50-00-0	Formaldehyde			4.9E+00	1.5E+00	5.1E+01
50-29-3	DDT, p,p'-		2.8E-04	1.2E-02	8.8E-03	
50-32-8	Benzo[a]pyrene	2.0E-04	1.3E-05		5.4E-03*	
51-28-5	Dinitrophenol 2,4-			4.9E-02		
53-70-3	Dibenz[a,h]anthracene		1.3E-05		3.8E-01*	
55-18-5	N-Nitrosodiethylamine		6.4E-07		4.3E-05	
56-23-5	Carbon tetrachloride	5.0E-03	7.4E-04	1.7E-02	7.6E-04	2.1E-02
56-38-2	Parathion (ethyl)			1.5E-01		
56-49-5	Methylcholanthrene 3-				1.2E-03	
56-53-1	Diethylstilbestrol		2.1E-08			
56-55-3	Benz[a]anthracene		8.0E-05		1.8E-02*	
57-24-9	Strychnine and salts			7.3E-03		
57-74-9	Chlordane	2.0E-03	2.8E-04	1.2E-02	1.5E-03	2.8E-02
57-97-6	Dimethylbenz[a]anthracene 7,12-				3.0E-03	
58-89-9	HCH (Lindane) gamma-	2.0E-04	7.4E-05	7.3E-03	1.6E-03	
58-90-2	Tetrachlorophenol 2,3,4,6-			7.3E-01		
60-29-7	Ethyl ether			4.9E+00		
60-51-5	Dimethoate			4.9E-03		
60-57-1	Dieldrin		6.0E-06	1.2E-03	1.0E-04	
62-38-4	Phenyl mercuric acetate			2.0E-03		
62-50-0	Ethyl methane sulfonate		3.3E-07			
62-53-3	Aniline (benzeneamine)		1.7E-02		2.2E+00	9.3E-01
62-75-9	N-Nitrosodimethylamine		1.9E-06	2.0E-04	4.0E-04	
64-18-6	Formic acid			4.9E+01		
67-56-1	Methanol			1.2E+01		1.5E+03
67-64-1	Acetone (2-propanone)			2.4E+00		1.5E+03
67-66-3	Chloroform			2.4E-01		3.3E-01
67-72-1	Hexachloroethane		6.9E-03	2.4E-02	3.3E-03	
68-12-2	N,N-Dimethyl formamide [DMF]			2.4E+00		7.1E+02
70-30-4	Hexachlorophene			7.3E-03		
71-36-3	Butanol			2.4E+00		
71-43-2	Benzene	5.0E-03	1.8E-03		1.6E-03	1.9E-01
71-55-6	Trichloroethane 1,1,1-	2.0E-01		6.9E+00		6.9E+00
72-20-8	Endrin	2.0E-03		7.3E-03		
72-43-5	Methoxychlor	4.0E-02		1.2E-01*		
72-54-8	DDD		4.0E-04			
72-55-9	DDE		2.8E-04			
74-83-9	Bromomethane (methyl bromide)			3.4E-02		1.5E-02
74-87-3	Chloromethane (methyl chloride)		7.4E-03		5.9E-03	2.6E-01
74-95-3	Methylene bromide (Dibromomethane)			2.4E-01		
75-00-3	Chloroethane [Ethyl chloride]					3.0E+01
75-01-4	Vinyl chloride	2.0E-03	1.3E-04	7.3E-02	2.5E-03	2.9E-01
75-05-8	Acetonitrile (methyl cyanide)					3.1E+00

CAS Number	Chemical Name	MCL (mg/L)	Ingestion HBNs		Inhalation HBNs	
			Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)	Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)
75-07-0	Acetaldehyde [Ethanal]				4.1E-02	2.2E-01
75-09-2	Methylene Chloride (Dichloromethane)	5.0E-03	1.3E-02	1.5E+00	2.8E-02	1.0E+01
75-15-0	Carbon disulfide			2.4E+00		1.9E+00
75-21-8	Ethylene oxide		9.5E-05		5.2E-04	4.1E-01
75-25-2	Tribromomethane (Bromoform)		1.2E-02	4.9E-01	1.9E-02	
75-27-4	Bromodichloromethane		1.6E-03	4.9E-01	8.0E-04	
75-34-3	Dichloroethane 1,1-			2.4E+00	7.4E-03	1.6E+00
75-35-4	Dichloroethylene 1,1-	7.0E-03	1.6E-04	2.2E-01	2.2E-04	2.1E-01
75-56-9	Propylene oxide [1,2-Epoxypropane]		4.0E-04		1.7E-02	4.9E-01
75-69-4	Trichlorofluoromethane (Freon 11)			7.3E+00		2.1E+00
75-71-8	Dichlorodifluoromethane (Freon 12)			4.9E+00		5.8E-01
76-13-1	Trichloro-1,2,2-trifluoro- ethane 1,1,2-			7.3E+02*		9.5E+01
76-44-8	Heptachlor	4.0E-04	2.1E-05	1.2E-02	1.5E-05	
77-47-4	Hexachlorocyclopentadiene	5.0E-02		1.5E-01		6.9E-04
78-59-1	Isophorone		1.0E-01	4.9E+00		5.3E+02
78-83-1	Isobutyl alcohol			7.3E+00		
78-87-5	Dichloropropane 1,2-	5.0E-03	1.4E-03	2.2E+00		1.4E-02
78-93-3	Methyl ethyl ketone			1.5E+01		3.3E+01
79-00-5	Trichloroethane 1,1,2-	5.0E-03	1.7E-03	9.8E-02	1.1E-03	
79-01-6	Trichloroethylene (1,1,2-Trichloroethylene)	5.0E-03	8.8E-03		6.8E-03	1.9E+00
79-06-1	Acrylamide		2.1E-05	4.9E-03	5.1E+00	
79-10-7	Acrylic acid [propenoic acid]			1.2E+01		1.5E+01
79-34-5	Tetrachloroethane 1,1,2,2-		4.8E-04	1.5E+00	5.0E-04	
79-46-9	Nitropropane 2-				2.3E-05	3.3E-01
80-62-6	Methyl methacrylate			3.4E+01		5.3E+00
82-68-8	Pentachloronitrobenzene (PCNB)		3.7E-04	7.3E-02		
83-32-9	Acenaphthene			1.5E+00		
84-66-2	Diethyl phthalate			2.0E+01		
84-74-2	Di-n-butyl phthalate			2.4E+00		
85-44-9	Phthalic anhydride			4.9E+01		1.3E+04*
85-68-7	Butyl benzyl phthalate			4.9E+00*		
86-30-6	N-Nitrosodiphenylamine		2.0E-02	4.9E-01	5.2E-01	
86-73-7	Fluorene			9.8E-01		
87-68-3	Hexachloro-1,3-butadiene		1.2E-03	7.3E-03	6.1E-04	
87-86-5	Pentachlorophenol	1.0E-03	8.0E-04	7.3E-01	5.4E+01	
88-06-2	Trichlorophenol 2,4,6-		8.8E-03		2.8E-01	
88-85-7	Butyl-4,6-dinitrophenol,2-sec-(Dinoseb)	7.0E-03		2.4E-02		
91-20-3	Naphthalene			4.9E-01		1.9E-02
91-94-1	Dichlorobenzidine 3,3'-		2.1E-04		4.9E+00*	
92-87-5	Benzidine		4.2E-07	7.3E-02	2.6E+00	
93-72-1	Trichlorophenoxy)propionic acid 2-(2,4,5-(Silvex)	5.0E-02		2.0E-01		
93-76-5	Trichlorophenoxyacetic acid 2,4,5-			2.4E-01		
94-59-7	Safrole		5.4E-04			
94-75-7	Dichlorophenoxyacetic acid 2,4-(2,4-D)	7.0E-02		2.4E-01		

CAS Number	Chemical Name	MCL (mg/L)	Ingestion HBNs		Inhalation HBNs	
			Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)	Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)
95-47-6	Xylene, o-			4.9E+01		1.4E+00
95-48-7	Cresol, o-			1.2E+00		8.8E+02
95-50-1	Dichlorobenzene1,2-	6.0E-01		2.2E+00		7.7E-01
95-53-4	Toluidine o-		4.0E-04		3.6E-02	
95-57-8	Chlorophenol 2-			1.2E-01		9.7E-03
95-65-8	3,4-Dimethylphenol			2.4E-02		
95-80-7	Toluenediamine 2,4-		3.0E-05		7.5E+00	
95-94-3	Tetrachlorobenzene 1,2,4,5-			7.3E-03		
95-95-4	Trichlorophenol 2,4,5-			2.4E+00		
96-12-8	Dibromo-3-chloropropane1,2-	2.0E-04	6.9E-05		7.9E-02	2.9E-03
96-18-4	Trichloropropane 1,2,3-		1.4E-05	1.5E-01		3.4E-02
96-45-7	Ethylene thiourea		8.8E-04	2.0E-03	1.6E+03	
97-63-2	Ethyl methacrylate			2.2E+00		
98-01-1	Furfural			7.3E-02		2.2E+01
98-82-8	Cumene			2.4E+00		1.3E+00
98-86-2	Acetophenone			2.4E+00		
98-95-3	Nitrobenzene			1.2E-02		1.5E-01
99-35-4	Trinitrobenzene (1,3,5-Trinitrobenzene) sym-			7.3E-01		
99-65-0	Dinitrobenzene 1,3-			2.4E-03		
100-41-4	Ethylbenzene	7.0E-01		2.4E+00	1.1E-02	3.3E+00
100-42-5	Styrene	1.0E-01		4.9E+00		3.6E+00
100-44-7	Benzyl chloride		5.7E-04		5.2E-04	
100-51-6	Benzyl alcohol			7.3E+00		
100-75-4	N-Nitrosopiperidine				8.7E-03	
105-67-9	Dimethylphenol 2,4-			4.9E-01		
106-42-3	Xylene, p-			4.9E+01		1.3E+00
106-44-5	Cresol, p-			1.2E-01		1.3E+03
106-46-7	Dichlorobenzene1,4-	7.5E-02	4.0E-03		1.3E-03	3.0E+00
106-47-8	Chloroaniline p-			9.8E-02		
106-49-0	Toluidine p-		5.1E-04			
106-88-7	1,2-Epoxybutane					2.4E-01
106-89-8	Epichlorohydrin		9.8E-03	4.9E-02	1.9E-01	6.0E-02
106-93-4	Ethylene dibromide (1,2-Dibromoethane)	5.0E-05	1.1E-06		8.4E-05	9.8E-04
106-99-0	1,3-Butadiene				4.0E-05	6.0E-02
107-02-8	Acrolein			4.9E-01		3.3E-04
107-05-1	Chloropropene, 3- (Allyl Chloride)				1.9E-03	3.0E-03
107-06-2	Dichloroethane1,2-	5.0E-03	1.1E-03		6.3E-04	1.0E+01
107-13-1	Acrylonitrile		1.8E-04	2.4E-02	1.0E-03	3.8E-02
107-18-6	Allyl alcohol			1.2E-01		
107-21-1	Ethylene glycol			4.9E+01		1.2E+04
108-05-4	Vinyl acetate			2.4E+01		1.2E+00
108-10-1	Methyl isobutyl ketone			2.0E+00		1.2E+00
108-38-3	Xylene, m-			4.9E+01		1.3E+00
108-39-4	Cresol, m-			1.2E+00		1.2E+03
108-45-2	Phenylenediamine, 1,3-			1.5E-01		

CAS Number	Chemical Name	MCL (mg/L)	Ingestion HBNs		Inhalation HBNs	
			Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)	Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)
108-88-3	Toluene	1.0E+00		4.9E+00		1.3E+00
108-90-7	Chlorobenzene	1.0E-01		4.9E-01		2.0E-01
108-93-0	Cyclohexanol			4.2E-04		3.9E-04
108-94-1	Cyclohexanone			1.2E+02		
108-95-2	Phenol			1.5E+01		9.0E+02
109-86-4	2-Methoxyethanol			2.4E-02		4.4E+02
110-00-9	Furan			2.4E-02		
110-49-6	2-Methoxyethanol acetate			4.9E-02		5.1E+02
110-54-3	n-Hexane			2.7E+02*		6.6E-01
110-80-5	Ethoxyethanol 2-			9.8E+00		2.9E+03
110-86-1	Pyridine			2.4E-02		1.4E+00
111-15-9	2-Ethoxyethanol acetate			7.3E+00		3.0E+02
111-44-4	Bis(2-chloroethyl)ether		8.8E-05		1.1E-03	
115-29-7	Endosulfan (Endosulfan I and II,mixture)			1.5E-01		
117-81-7	Bis(2-ethylhexyl)phthalate	6.0E-03	6.9E-03	4.9E-01*	2.8E+01*	1.8E+02*
117-84-0	Di-n-octyl phthalate			4.9E-01*		
118-74-1	Hexachlorobenzene	1.0E-03	6.0E-05	2.0E-02*	3.6E-05	
119-90-4	Dimethoxybenzidine 3,3'-		6.9E-03			
119-93-7	Dimethylbenzidine 3,3'-		1.0E-05			
120-12-7	Anthracene			7.3E+00*		
120-82-1	Trichlorobenzene 1,2,4-	7.0E-02		2.4E-01		8.3E-01
120-83-2	Dichlorophenol 2,4-			7.3E-02		
121-14-2	Dinitrotoluene 2,4-		1.4E-04	4.9E-02	8.1E-01	
121-44-8	Triethylamine					1.1E-01
122-39-4	Diphenylamine			6.1E-01		
122-66-7	1,2-Diphenylhydrazine		1.2E-04		2.0E-02	
123-91-1	Dioxane 1,4-		8.8E-03		1.8E-01	1.1E+03
124-48-1	Chlorodibromomethane		1.1E-03	4.9E-01	7.5E-04	
126-72-7	Tris(2,3-dibromopropyl)phosphate		9.9E-06			
126-98-7	Methacrylonitrile			2.4E-03		6.5E-03
126-99-8	Chloro-1,3-butadiene 2-(Chloroprene)			4.9E-01		2.2E-02
127-18-4	Tetrachloroethylene	5.0E-03	1.9E-03	2.4E-01	2.1E-02	9.4E-01
129-00-0	Pyrene			7.3E-01*		
131-11-3	Dimethyl phthalate					
137-26-8	Thiram [Thiuram]			1.2E-01		
141-78-6	Ethyl acetate			2.2E+01		
143-50-0	Kepone			1.2E-02		
152-16-9	Octamethyl pyrophosphoramidate			4.9E-02		
156-59-2	Dichloroethylene cis-1,2-	7.0E-02		2.4E-01		
156-60-5	Dichloroethylene trans-1,2-	1.0E-01		4.9E-01		
193-39-5	Indeno{1,2,3-cd}pyrene		8.0E-05*		3.8E-02*	
205-99-2	Benzo{b}fluoranthene		8.0E-05		6.3E-04	
206-44-0	Fluoranthene			9.8E-01*		
218-01-9	Chrysene		8.0E-04		7.3E-03*	
298-00-0	Methyl parathion			6.1E-03		
298-02-2	Phorate			4.9E-03		

CAS Number	Chemical Name	MCL (mg/L)	Ingestion HBNs		Inhalation HBNs	
			Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)	Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)
298-04-4	Disulfoton			9.8E-04		
309-00-2	Aldrin		5.7E-06	7.3E-04	1.0E-05	
319-84-6	HCH alpha-		1.5E-05	2.0E-01	3.6E-04	
319-85-7	HCH beta-		5.4E-05		1.7E-02	
510-15-6	Chlorobenzilate		3.6E-04	4.9E-01	1.2E+00	
542-75-6	Dichloropropene 1,3-(mixture of isomers)		9.7E-04	7.3E-01	2.9E-03	6.1E-02
606-20-2	Dinitrotoluene 2,6-		1.4E-04	2.4E-02		
608-93-5	Pentachlorobenzene			2.0E-02		
621-64-7	N-Nitroso-di-n-propylamine		1.4E-05		1.5E-03	
630-20-6	Tetrachloroethane 1,1,1,2-		3.7E-03	7.3E-01	1.9E-03	
924-16-3	N-Nitroso-di-n-butylamine		1.8E-05		2.0E-05	
930-55-2	N-Nitrosopyrrolidine		4.6E-05		9.2E-01	
1024-57-3	Heptachlor epoxide	2.0E-04	1.1E-05	3.2E-04	2.8E-04	
1319-77-3	Cresols (total)			1.2E+00		1.1E+03
1330-20-7	Xylenes (total)	1.0E+01		4.9E+01		1.4E+00
1336-36-3	Polychlorinated biphenyls (Aroclors)	5.0E-04	2.4E-04	4.9E-04	1.4E-04	
1634-04-4	Methyl tert-butyl ether [MTBE]					1.7E+01
1746-01-6	Tetrachlorodibenzo-p-dioxin 2,3,7,8-[2,3,7,8-TCDD]	3.0E-08	6.4E-10	2.4E-08	2.2E-09	
2303-16-4	Diallate		1.6E-03			
3689-24-5	Tetraethyl dithiopyrophosphate (Sulfotep)			1.2E-02		
7439-92-1	Lead	0.015**				
7439-96-5	Manganese			1.2E+00		
7439-97-6	Mercury	2.0E-03		2.4E-03		7.0E-04
7439-98-7	Molybdenum			1.2E-01		
7440-02-0	Nickel			4.9E-01		
7440-22-4	Silver			1.2E-01		
7440-28-0	Thallium	2.0E-03		2.0E-03		
7440-36-0	Antimony	6.0E-03		9.8E-03		
7440-38-2	Arsenic	5.0E-02	6.4E-05	7.3E-03		
7440-39-3	Barium	2.0E+00		1.7E+00		
7440-41-7	Beryllium	4.0E-03		4.9E-02		
7440-43-9	Cadmium	5.0E-03		1.2E-02		
7440-48-4	Cobalt			4.9E-01		
7440-50-8	Copper	1.3**				
7440-62-2	Vanadium			1.7E-01		
7440-66-6	Zinc			7.3E+00		
7782-49-2	Selenium	5.0E-02		1.2E-01		
8001-35-2	Toxaphene (chlorinated camphenes)	3.0E-03	8.8E-05		3.6E-03	
10061-01-5	Dichloropropene cis-1,3-		9.7E-04	7.3E-01	3.3E-03	7.0E-02
10061-02-6	Dichloropropene trans-1,3-		9.7E-04	7.3E-01	3.5E-03	7.5E-02
10595-95-6	N-Nitrosomethylethylamine		4.4E-06		4.5E-03	
16065-83-1	Chromium (III)	1.0E-01		3.7E+01		
16984-48-8	Fluoride	4.0E+00		1.5E+00		
18540-29-9	Chromium (VI)	1.0E-01		7.3E-02		
23950-58-5	Pronamide			1.8E+00		

CAS Number	Chemical Name	MCL (mg/L)	Ingestion HBNs		Inhalation HBNs	
			Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)	Cancer HBN (mg/L)	Non-Cancer HBN (mg/L)
30402-15-4	Pentachlorodibenzofurans [PeCDFs]		1.3E-09		6.3E-08	
34465-46-8	Hexachlorodibenzo-p-dioxins [HxCDDs]		6.4E-09		1.4E-07	
36088-22-9	Pentachlorodibenzo-p-dioxins [PeCDDs]		6.4E-10		6.0E-08	
39638-32-9	Bis(2-chloroisopropyl)ether		1.4E-03	9.8E-01	5.9E-03	
51207-31-9	Tetrachlorodibenzofuran 2,3,7,8- [2,3,7,8-TCDF]		6.4E-09		1.0E-07	

Key:

CASRN = Chemical Abstract Service registry number.

* = Value exceeds contaminant's water solubility (see Section 3.2.1.2)

** = Value is a drinking water "action level" as specified by 40 CFR 141.32(e)(13) and (14).

3.3 References for Section 3.0

Coburn, J. 1996. Memo to Dana Greenwood on Emission Flux Equations for Showering, July 1.

Little, J.C. 1992a. Applying the two resistance theory to contaminant volatilization in showers. *Environmental Science and Technology* 26(7):1341-1349.

Little, J.C. 1992b. Applying the two resistance theory to contaminant volatilization in showers. *Environmental Science and Technology* 26(4); 836-837.

McKone, T.E. 1987. Human exposure to volatile organic compounds in household tap water: The indoor inhalation pathway. *Environmental Science and Technology* 21:1194-1201.

USEPA. 1991. *Risk Assessment Guidance for Superfund: Volume 1 - Human Health Evaluation Manual (Part B, Development of Risk-Based Preliminary Goals)*. EPA/540/R-92/003. Interim Draft. Office of Emergency and Remedial Response, USEPA, Washington, DC.

USEPA. 1992. 57 Federal Register 22888. Final Guidelines for Exposure Assessment. U.S. Environmental Protection Agency. May 29.

USEPA. 1996. *Soil Screening Guidance: Technical Background Document*. EPA/540/R95/128. Office of Solid Waste and Emergency Response. May.

USEPA. 1997a. *Exposure Factors Handbook, Volume I, General Factors*. EPA/600/P-95/002Fa. Office of Research and Development, Washington, DC.

USEPA. 1997b. *Exposure Factors Handbook, Volume II, Food Ingestion Factors*. EPA/600/P-95/002Fb. Office of Research and Development, Washington, DC.

USEPA. 1997c. *Exposure Factors Handbook, Volume III, Activity Factors*. EPA/600/P-95/002Fc. Office of Research and Development, Washington, DC.

USEPA. 2000. *Volatilization Rates from Water to Indoor Air, Phase II*. EPA/600/R-00/096. National Center for Environmental Assessment–Washington Office, Office of Research and Development, Washington, DC. October.

Attachment A

Shower Equations

Equation A-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 Equation A-12
ShowerStallTime	Time in shower stall after showering (min)	Provided in Equation A-12
T_bathroom	Time spent in bathroom, not in shower (min)	Provided in Equation A-12

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

Equation Equation A-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 Equation A-12
ShowerTime	Duration of shower (min)	Provided in Equation A-12

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

Equation A-3. Dimensionless Henry's law constant

$$H_{prime} = HLC_{coef} \times HLC$$

$$HLC_{coef} = \frac{1}{R \times Temp}$$

Name	Description	Value
Hprime	Dimensionless Henry's law constant (dimensionless)	Calculated above
HLCcoef	Coefficient to Henry's law constant (dimensionless)	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 A-4. Dimensionless overall mass transfer coefficient

$$N = Kol \times AVRatio \times DropResTime$$

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

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

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 A-5
DropResTime	Residence time for falling drops (s)	Calculated above
DropDiam	Drop diameter (cm)	Provided in Equation A-12
NozHeight	Nozzle height (m)	Provided in Equation A-12
DropVel	Drop terminal velocity (cm/s)	Provided in Equation A-12
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 $N = Kol \times A/Q1$ where A is the total surface area for mass transfer and Q1 is water flow in volume per time.

Equation A-5. Overall mass transfer coefficient

$$K_{ol} = \beta \times \left(\frac{2.5}{D_w^{2/3}} + \frac{1}{D_a^{2/3} \times H_{prime}} \right)^{-1}$$

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
Hprime	Dimensionless Henry's law constant (dimensionless)	Calculated in Equation A-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 A-6. Contaminant mass emitted in the shower for a given time step

For $E_t > E_{max}$,

$$E_s = E_{max}$$

For $E_t \leq E_{max}$,

$$E_s = E_t$$

Where,

$$E_t = C_{in} \times ShowerRate \times t_s \times f_{em}$$

$$E_{max} = (y_{eq} - y_{s,t}) \times V_s \times 1000$$

Name	Description	Value
Es	Contaminant mass emitted in the shower for a given time step (mg)	Calculated above
E _{max}	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
y _{eq}	Gas-phase constituent concentration in equilibrium between water and air (mg/L)	H _{prime} x C _{in}
y _{s, t}	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated from last time step
V _s	Volume of shower (m ³)	Provided in Equation A-12
C _{in}	Liquid-phase constituent concentration in the incoming water (mg/L)	Provided in Equation A-12
ShowerRate	Rate of flow from showerhead (L/min)	Provided in Equation A-12
t _s	Time step (min)	0.2
f _{em}	Fraction of constituent emitted from a droplet (dimensionless)	Calculated in Equation A-7
H _{prime}	Dimensionless Henry's law constant (dimensionless)	Calculated in Equation A-3
1000	Conversion factor (L/m ³)	Conversion factor

The above equations are used to determine the mass of contaminant 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 (E_{max}), the mass is set to the amount that results in the air concentration at equilibrium.

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

$$f_{em} = (1 - F_{sat}) \times (1 - e^{-N})$$

Name	Description	Value
fem	Fraction of constituent emitted from a droplet (dimensionless)	Calculated above
Fsat	Fraction of gas-phase saturation (dimensionless)	Calculated in Equation A-8
N	Dimensionless overall mass transfer coefficient (dimensionless)	Calculated in Equation A-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 $y_{s_max}/m = C_{in}$ and $f_{sat} = y_s/y_{s_max} = y_s/(m \times C_{in})$.

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

$$F_{sat} = \frac{y_{s,t}}{y_{eq}}$$

Name	Description	Value
Fsat	Fraction of gas-phase saturation in shower (dimensionless)	Calculated above
y _{eq}	Gas-phase contaminant concentration in equilibrium between water and air (mg/L)	H _{prime} x C _{in}
y _{s, t}	Current gas-phase contaminant concentration in air (mg/L)	Calculated in Equation A-9 (as y _{s, t+ts} for previous time step)
H _{prime}	Dimensionless Henry's law constant (dimensionless)	Calculated in Equation A-3
C _{in}	Constituent concentration in incoming water (mg/L)	Provided in Equation A-12

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

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

Name	Description	Value
$y_{s,t+ts}$	Gas-phase constituent concentration in the shower at end of time step (mg/L)	Calculated above
$y_{s,t}$	Gas-phase constituent concentration in the shower at the beginning of time step (mg/L)	Calculated from last time step
$y_{b,t}$	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
E_s	Mass emitted in the shower for a given time step (mg)	Calculated in Equation A-6
Q_{sb}	Volumetric exchange rate between the shower and the bathroom (L/min)	Provided in Equation A-12
V_s	Volume of shower (m ³)	Provided in Equation A-12
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). E_s 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 A-10. Gas-phase constituent concentration in the bathroom at end of time step

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

Name	Description	Value
$y_{b,t+ts}$	Gas-phase constituent concentration in the bathroom at end of time step (mg/L)	Calculated above
$y_{b,t}$	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
$y_{s,t+ts}$	Gas-phase constituent concentration in the shower at the end of time step (mg/L)	Calculated in Equation A-9
$y_{h,t}$	Gas-phase constituent concentration in the house at the beginning of time step (mg/L)	Assumed de minimus, zero
Q_{sb}	Volumetric exchange rate between the shower and the bathroom (L/min)	Provided in Equation A-12
Q_{bh}	Volumetric exchange rate between the bathroom and the house (L/min)	Provided in Equation A-12
V_b	Volume of bathroom (m ³)	Provided in Equation A-12
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 A-11. Average daily concentration in indoor air

$$C_{air_indoor} = \frac{(C_{air_shower} \times ShowerResTime) + (C_{air_bathroom} \times T_{bathroom})}{1440}$$

$$C_{air_shower} = \frac{\sum [(y_{s,t+ts} + y_{s,t}) / 2] \times 1000}{n_s}$$

$$C_{air_bathroom} = \frac{\sum [(y_{b,t+ts} + y_{b,t}) / 2] \times 1000}{n_b}$$

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 A-2
T_bathroom	Time spent in bathroom, not in shower (min)	Provided in Equation A-12
ys, t	Gas-phase constituent concentration in the shower 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 A-9
yb, t	Gas-phase constituent concentration in the bathroom at the beginning of time step (mg/L)	Calculated from last time step
yb, t+ts	Gas-phase constituent concentration in the bathroom at the end of time step (mg/L)	Calculated in Equation A-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)	
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 contaminants in the shower and bathroom.

Attachment B

Contaminant-specific Chemical and Physical Properties for the Shower Model

Attachment B

Contaminant-specific Chemical and Physical Properties for the Shower Model

To calculate inhalation HBNs, the shower model requires input of several chemical-specific properties, including Henry's law constant (*HLC*), solubility (*Sol*), 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 B-1 (at the end of this attachment) lists by contaminant the chemical-specific properties used to calculate inhalation HBNs, along with the data source for each value.

B.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)* (USEPA, 2000). We used the *Mercury Study Report to Congress* (USEPA, 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 contaminants.

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.

B.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) (USEPA, 1997b);
2. CHEMFATE Chemical Search (SRC, 1999);
3. Hazardous Substances Data Bank (HSDB) (USNLM, 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).

B.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).

B.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 (USEPA, 2001):

$$D_w = 0.0001518 \left(\frac{T + 27316}{29816} \right) \left(\frac{MW}{\rho} \right)^{-0.6}$$

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 (Process Coefficients)* (USEPA, 1987), which only requires molecular weight:

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

where

D_w = diffusion coefficient in water (cm²/s)
 MW = molecular weight (g/mol).

B.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 USEPA (1987). Equation 17-5 in WATER9 calculates diffusivity in air as follows:

$$D_a = \frac{0.0029(T + 273.16)^{1.5} \sqrt{0.034 + \frac{1}{MW} \{1 - 0.000015MW^2\}}}{\left[\left(\frac{MW}{2.5\rho} \right)^{0.333} + 18 \right]^2}$$

where

D_a = diffusion coefficient in air (cm²/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):

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

where

D_a = diffusion coefficient in air (cm²/s)
 MW = molecular weight (g/mol).

For dioxins and furans, we used an equation from the Dioxin Reassessment (USEPA, 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 (cm²/s)
- D_b = diffusion coefficient of diphenyl at 25 degrees C (0.068 cm²/s)
- MW_a = molecular weight of constituent (g/mole)
- MW_b = molecular weight of diphenyl (154 g/mole).

Table B-1. Contaminant-specific Chemical and Physical Properties

Contaminant	CASRN	D _a (cm ² /s)	D _w (cm ² /s)	HLC	
				(atm·m ³ /mol)	SoI (mg/L)
Acetaldehyde (ethanal)	75-07-0	1.28E-01 e	1.35E-05 e	7.89e-05 a	1.00e+06 a
Acetone (2-propanone)	67-64-1	1.06E-01 e	1.15E-05 e	3.88e-05 a	1.00e+06 a
Acetonitrile (methyl cyanide)	75-05-8	1.34E-01 e	1.41E-05 e	3.46e-05 a	1.00e+06 a
Acrolein	107-02-8	1.12E-01 e	1.22E-05 e	1.22e-04 a	2.13e+05 a
Acrylamide	79-06-1	1.07E-01 e	1.26E-05 e	1.00e-09 a	6.40e+05 a
Acrylic acid (propenoic acid)	79-10-7	1.03E-01 e	1.20E-05 e	1.17e-07 a	1.00e+06 a
Acrylonitrile	107-13-1	1.14E-01 e	1.23E-05 e	1.03e-04 a	7.40e+04 a
Aldrin	309-00-2	2.28E-02 e	5.84E-06 e	1.70e-04 a	1.80e-01 a
Aniline (benzeneamine)	62-53-3	8.30E-02 e	1.01E-05 e	1.90e-06 a	3.60e+04 a
Benz(a)anthracene	56-55-3	5.09E-02 b	5.89E-06 b	3.35e-06 a	9.40e-03 a
Benzene	71-43-2	8.95E-02 e	1.03E-05 e	5.55e-03 a	1.75e+03 a
Benidine	92-87-5	3.55E-02 e	7.59E-06 e	3.88e-11 a	5.00e+02 a
Benzo(a)pyrene	50-32-8	2.55E-02 e	6.58E-06 e	1.13e-06 a	1.62e-03 a
Benzo(b)fluoranthene	205-99-2	4.76E-02 b	5.51E-06 b	1.11e-04 a	1.50e-03 a
Benzyl chloride	100-44-7	6.34E-02 e	8.81E-06 e	4.15e-04 a	5.25e+02 a
Bis(2-ethylhexyl)phthalate	117-81-7	1.73E-02 e	4.18E-06 e	1.02e-07 a	3.40e-01 a
Bis(2-chloroethyl)ether	111-44-4	5.67E-02 e	8.71E-06 e	1.80e-05 a	1.72e+04 a
Bis(2-chloroisopropyl)ether	39638-32-9	4.01E-02 e	7.40E-06 e	1.34e-04 d	1.31e+03 a
Bromodichloromethane	75-27-4	5.63E-02 e	1.07E-05 e	1.60e-03 a	6.74e+03 a
Bromomethane (methyl bromide)	74-83-9	1.00E-01 e	1.35E-05 e	6.24e-03 a	1.52e+04 a
Butadiene, 1,3-	106-99-0	1.00E-01 e	1.03E-05 e	7.36e-02 a	7.35e+02 a
Carbon tetrachloride	56-23-5	5.71E-02 e	9.78E-06 e	3.04e-02 a	7.93e+02 a
Carbon disulfide	75-15-0	1.06E-01 e	1.30E-05 e	3.03e-02 a	1.19e+03 a
Chlordane	57-74-9	2.15E-02 e	5.45E-06 e	4.86e-05 a	5.60e-02 a
Chloro-1,3-butadiene, 2- (Chloroprene)	126-99-8	8.41E-02 e	1.00E-05 e	1.19e-02 f	1.74e+03 a
Chlorobenzene	108-90-7	7.21E-02 e	9.48E-06 e	3.70e-03 a	4.72e+02 a
Chlorobenzilate	510-15-6	2.18E-02 e	5.48E-06 e	7.24e-08 f	1.11e+01 a
Chlorodibromomethane	124-48-1	3.66E-02 e	1.06E-05 e	7.83e-04 a	2.60e+03 a
Chloroethane (ethyl chloride)	75-00-3	1.04E-01 e	1.16E-05 e	8.82e-03 a	5.68e+03 a
Chloroform	67-66-3	7.70E-02 e	1.09E-05 e	3.67e-03 a	7.92e+03 a
Chloromethane (methyl chloride)	74-87-3	1.24E-01 e	1.36E-05 e	8.82e-03 a	5.33e+03 a
Chlorophenol, 2-	95-57-8	6.61E-02 e	9.48E-06 e	3.91e-04 a	2.20e+04 a
Chloropropene, 3- (allyl chloride)	107-05-1	9.36E-02 e	1.08E-05 e	1.10e-02 a	3.37e+03 a
Chrysene	218-01-9	2.61E-02 e	6.75E-06 e	9.46e-05 a	1.60e-03 a
Cresol, o-	95-48-7	7.59E-02 e	9.86E-06 e	1.20e-06 a	2.60e+04 a
Cresol, m-	108-39-4	7.29E-02 e	9.32E-06 e	8.65e-07 a	2.27e+04 a

(continued)

Table B-1. (continued)

Contaminant	CASRN	D _a (cm ² /s)	D _w (cm ² /s)	HLC	
				(atm·m ³ /mol)	Sol (mg/L)
Cresol, p-	106-44-5	7.24E-02 e	9.24E-06 e	7.92e-07 a	2.15e+04 a
Cresols (total)	1319-77-3	7.37E-02 e	9.48E-06 e	9.52e-07 a	2.34e+04 a
Cumene	98-82-8	6.02E-02 e	7.85E-06 e	1.16e+00 a	6.13e+01 a
Cyclohexanol	108-93-0	7.59E-02 e	9.35E-06 e	1.02e-04 f	4.30e+04 f
DDT, p,p'-	50-29-3	1.83E-02 e	4.44E-06 e	8.10e-06 a	2.50e-02 a
Dibenz(a,h)anthracene	53-70-3	2.36E-02 e	6.02E-06 e	1.47e-08 a	2.49e-03 a
Dibromo-3-chloropropane, 1,2-	96-12-8	3.21E-02 e	8.90E-06 e	1.47e-04 a	1.23e+03 a
Dichlorobenzene, 1,2-	95-50-1	5.62E-02 e	8.92E-06 e	1.90e-03 a	1.56e+02 a
Dichlorobenzene, 1,4-	106-46-7	5.50E-02 e	8.68E-06 e	2.40e-03 a	7.38e+01 a
Dichlorobenzidine, 3,3'-	91-94-1	4.75E-02 b	5.50E-06 b	4.00e-09 a	3.11e+00 a
Dichlorodifluoromethane (Freon 12)	75-71-8	7.60E-02 e	1.08E-05 e	3.43e-01 a	2.80e+02 a
Dichloroethane, 1,1-	75-34-3	8.36E-02 e	1.06E-05 e	5.62e-03 a	5.06e+03 a
Dichloroethane, 1,2-	107-06-2	8.54E-02 e	1.09E-05 e	9.79e-04 a	8.52e+03 a
Dichloroethylene, 1,1-	75-35-4	8.63E-02 e	1.10E-05 e	2.61e-02 a	2.25e+03 a
Dichloropropane, 1,2-	78-87-5	7.33E-02 e	9.73E-06 e	2.80e-03 a	2.80e+03 a
Dichloropropene, trans-1,3-	10061-02-6	7.63E-02 e	1.01E-05 e	1.80e-03 i	2.72e+03 a
Dichloropropene, 1,3- (isomer mixture)	542-75-6	7.63E-02 e	1.01E-05 e	1.77e-02 a	2.80e+03 a
Dichloropropene, cis-1,3-	10061-01-5	7.65E-02 e	1.02E-05 e	2.40e-03 i	2.72e+03 a
Dieldrin	60-57-1	2.33E-02 e	6.01E-06 e	1.51e-05 a	1.95e-01 a
Dimethyl formamide, N,N- (DMF)	68-12-2	9.72E-02 e	1.12E-05 e	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 a	2.50e-02 a
Dinitrotoluene, 2,4-	121-14-2	3.75E-02 e	7.90E-06 e	9.26e-08 a	2.70e+02 a
Dioxane, 1,4-	123-91-1	8.74E-02 e	1.05E-05 e	4.80e-06 a	1.00e+06 a
Diphenylhydrazine, 1,2-	122-66-7	0.0343 e	7.25E-06 e	1.53e-06 a	6.80e+01 a
Epichlorohydrin	106-89-8	0.0888 e	1.11E-05 e	3.04e-05 a	6.59e+04 a
Epoxybutane, 1,2-	106-88-7	9.32E-02 e	1.05E-05 e	1.80e-04 f	9.50e+04 f
Ethoxyethanol acetate, 2-	111-15-9	5.70E-02 e	7.98E-06 e	1.80e-06 i	2.29e+05 i
Ethoxyethanol, 2-	110-80-5	8.19E-02 e	9.76E-06 e	1.23e-07 a	1.00e+06 a
Ethylbenzene	100-41-4	6.86E-02 e	8.48E-06 e	7.88e-03 a	1.69e+02 a
Ethylene dibromide (1,2-dibromoethane)	106-93-4	4.31E-02 e	1.05E-05 e	7.43e-04 a	4.18e+03 a
Ethylene glycol	107-21-1	1.17E-01 e	1.36E-05 e	6.00e-08 a	1.00e+06 a
Ethylene thiourea	96-45-7	8.69E-02 b	1.01E-05 b	3.08e-10 a	6.20e+04 a
Ethylene oxide	75-21-8	1.34E-01 e	1.46E-05 e	1.48e-04 f	1.00e+06 g
Formaldehyde	50-00-0	1.67E-01 e	1.74E-05 e	3.36e-07 a	5.50e+05 a
Furfural	98-01-1	8.53E-02 e	1.07E-05 e	4.00e-06 a	1.10e+05 a
HCH, gamma- (Lindane)	58-89-9	2.74E-02 e	7.30E-06 e	1.40e-05 a	6.80e+00 a

(continued)

Table B-1. (continued)

Contaminant	CASRN	D _a (cm ² /s)	D _w (cm ² /s)	HLC	
				(atm·m ³ /mol)	Sol (mg/L)
HCH, beta-	319-85-7	0.0277 e	7.40E-06 e	7.43e-07 a	2.40e-01 a
HCH, alpha-	319-84-6	2.75E-02 e	7.35E-06 e	1.06e-05 a	2.00e+00 a
Heptachlor epoxide	1024-57-3	2.19E-02 e	5.58E-06 e	9.50e-06 a	2.00e-01 a
Heptachlor	76-44-8	2.23E-02 e	5.70E-06 e	1.10e-03 a	1.80e-01 a
Hexachloro-1,3-butadiene	87-68-3	2.67E-02 e	7.03E-06 e	8.15e-03 a	3.23e+00 a
Hexachlorobenzene	118-74-1	2.90E-02 e	7.85E-06 e	1.32e-03 a	5.00e-03 a
Hexachlorocyclopentadiene	77-47-4	2.72E-02 e	7.22E-06 e	2.70e-02 a	1.80e+00 a
Hexachlorodibenzo-p-dioxins (HxCDDs)	34465-46-8	4.27E-02 j	4.12E-06 b	1.10e-05 c	4.40e-06 c
Hexachlorodibenzofurans (HxCDFs)	55684-94-1	4.36E-02 j	4.23E-06 b	1.10e-05 c	1.30e-05 c
Hexachloroethane	67-72-1	3.21E-02 e	8.89E-06 e	3.89e-03 a	5.00e+01 a
Hexane, n-	110-54-3	7.28E-02 e	8.12E-06 e	1.43e-02 a	1.24e+01 a
Indeno(1,2,3-cd)pyrene	193-39-5	4.48E-02 b	5.19E-06 b	1.60e-06 a	2.20e-05 a
Isophorone	78-59-1	5.25E-02 e	7.53E-06 e	6.64e-06 a	1.20e+04 a
Mercury	7439-97-6	7.15E-02 e	3.01E-05 e	7.10e-03 k	5.62e-02 h
Methacrylonitrile	126-98-7	9.64E-02 e	1.06E-05 e	2.47e-04 a	2.54e+04 a
Methanol	67-56-1	1.58E-01 e	1.65E-05 e	4.55e-06 a	1.00e+06 a
Methoxyethanol acetate, 2-	110-49-6	6.59E-02 e	8.71E-06 e	3.11e-07 d	1.00e+06 i
Methoxyethanol, 2-	109-86-4	0.0952 e	1.10E-05 e	8.10e-08 f	1.00e+06 g
Methyl methacrylate	80-62-6	7.53E-02 e	9.25E-06 e	3.37e-04 a	1.50e+04 a
Methyl tert-butyl ether (MTBE)	1634-04-4	7.55E-02 e	8.63E-06 e	5.87e-04 f	5.13e+04 f
Methyl isobutyl ketone	108-10-1	6.98E-02 e	8.36E-06 e	1.38e-04 a	1.90e+04 a
Methyl ethyl ketone	78-93-3	9.17E-02 e	1.02E-05 e	5.59e-05 a	2.23e+05 a
Methylcholanthrene, 3-	56-49-5	2.41E-02 e	6.14E-06 e	9.40e-07 a	3.23e-03 a
Methylene chloride (dichloromethane)	75-09-2	9.99E-02 e	1.25E-05 e	2.19e-03 a	1.30e+04 a
N-Nitrosomethylethylamine	10595-95-6	8.41E-02 e	9.99E-06 e	1.40e-06 i	1.97e+04 a
N-Nitrosodimethylamine	62-75-9	9.88E-02 e	1.15E-05 e	1.20e-06 a	1.00e+06 a
N-Nitrosopiperidine	100-75-4	6.99E-02 e	9.18E-06 e	2.80e-07 a	7.65e+04 a
N-Nitrosodiphenylamine	86-30-6	2.84E-02 e	7.19E-06 e	5.00e-06 a	3.51e+01 a
N-Nitrosodiethylamine	55-18-5	7.38E-02 e	9.13E-06 e	3.63e-06 a	9.30e+04 a
N-Nitroso-di-n-butylamine	924-16-3	4.22E-02 e	6.83E-06 e	3.16e-04 a	1.27e+03 a
N-Nitrosopyrrolidine	930-55-2	8.00E-02 e	1.01E-05 e	1.20e-08 a	1.00e+06 a
N-Nitroso-di-n-propylamine	621-64-7	5.64E-02 e	7.76E-06 e	2.25e-06 a	9.89e+03 a
Naphthalene	91-20-3	6.05E-02 e	8.38E-06 e	4.83e-04 a	3.10e+01 a
Nitrobenzene	98-95-3	6.81E-02 e	9.45E-06 e	2.40e-05 a	2.09e+03 a
Nitropropane, 2-	79-46-9	8.47E-02 e	1.02E-05 e	1.23e-04 a	1.70e+04 a

(continued)

Table B-1. (continued)

Contaminant	CASRN	D _a (cm ² /s)	D _w (cm ² /s)	HLC	
				(atm·m ³ /mol)	Sol (mg/L)
Pentachlorodibenzo-p-dioxins (PeCDDs)	36088-22-9	4.47E-02 j	4.38E-06 b	2.60e-06 c	1.18e-04 c
Pentachlorodibenzofurans (PeCDFs)	30402-15-4	4.57E-02 j	4.51E-06 b	5.00e-06 c	2.40e-04 c
Pentachlorophenol	87-86-5	2.95E-02 e	8.01E-06 e	2.44e-08 a	1.95e+03 a
Phenol	108-95-2	8.34E-02 e	1.03E-05 e	3.97e-07 a	8.28e+04 a
Phthalic anhydride	85-44-9	5.95E-02 e	9.75E-06 e	1.63e-08 a	6.20e+03 a
Polychlorinated biphenyls (Aroclors)	1336-36-3	2.33E-02 e	5.98E-06 e	2.60e-03 a	7.00e-02 a
Propylene oxide (1,2-epoxypropane)	75-56-9	1.10E-01 e	1.21E-05 e	1.23e-04 f	4.05e+05 f
Pyridine	110-86-1	9.31E-02 e	1.09E-05 e	8.88e-06 a	1.00e+06 a
Styrene	100-42-5	7.13E-02 e	8.81E-06 e	2.75e-03 a	3.10e+02 a
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 c	1.93e-05 c
Tetrachlorodibenzofurans (TCDFs)*	55722-27-5	4.82E-02 j	4.84E-06 b	1.40e-05 c	4.20e-04 c
Tetrachloroethane, 1,1,2,2-	79-34-5	4.89E-02 e	9.29E-06 e	3.45e-04 a	2.97e+03 a
Tetrachloroethane, 1,1,1,2-	630-20-6	4.82E-02 e	9.10E-06 e	2.42e-03 a	1.10e+03 a
Tetrachloroethylene	127-18-4	5.05E-02 e	9.45E-06 e	1.84e-02 a	2.00e+02 a
Toluene	108-88-3	7.80E-02 e	9.23E-06 e	6.64e-03 a	5.26e+02 a
Toluenediamine 2,4-	95-80-7	7.72E-02 b	8.94E-06 b	7.92e-10 a	3.37e+04 a
Toluidine, o-	95-53-4	7.24E-02 e	9.18E-06 e	2.72e-06 a	1.66e+04 a
Toxaphene (chlorinated camphenes)	8001-35-2	2.16E-02 e	5.48E-06 e	6.00e-06 a	7.40e-01 a
Tribromomethane (bromoform)	75-25-2	3.58E-02 e	1.04E-05 e	5.35e-04 a	3.10e+03 a
Trichloro-1,2,2-trifluoro-ethane, 1,1,2-	76-13-1	3.76E-02 e	8.59E-06 e	4.81e-01 a	1.70e+02 a
Trichlorobenzene, 1,2,4-	120-82-1	3.96E-02 e	8.40E-06 e	1.42e-03 a	3.46e+01 a
Trichloroethane, 1,1,2-	79-00-5	6.69E-02 e	1.00E-05 e	9.13e-04 a	4.42e+03 a
Trichloroethane, 1,1,1-	71-55-6	6.48E-02 e	9.60E-06 e	1.72e-02 a	1.33e+03 a
Trichloroethylene (TCE)	79-01-6	6.87E-02 e	1.02E-05 e	1.03e-02 a	1.10e+03 a
Trichlorofluoromethane (Freon 11)	75-69-4	6.55E-02 e	1.01E-05 e	9.70e-02 a	1.10e+03 a
Trichlorophenol, 2,4,6-	88-06-2	3.14E-02 e	8.09E-06 e	7.79e-06 a	8.00e+02 a
Trichloropropane, 1,2,3-	96-18-4	5.75E-02 e	9.24E-06 e	4.09e-04 a	1.75e+03 a
Triethylamine	121-44-8	6.63E-02 e	7.84E-06 e	1.38e-04 f	5.50e+04 f
Vinyl acetate	108-05-4	8.51E-02 e	1.00E-05 e	5.11e-04 a	2.00e+04 a
Vinyl chloride	75-01-4	1.07E-01 e	1.20E-05 e	2.70e-02 a	2.76e+03 a
Xylene, p-	106-42-3	6.84E-02 e	8.45E-06 e	7.66e-03 a	1.85e+02 a
Xylene, o-	95-47-6	6.91E-02 e	8.56E-06 e	5.19e-03 a	1.78e+02 a
Xylene, m-	108-38-3	6.85E-02 e	8.47E-06 e	7.34e-03 a	1.61e+02 a
Xylenes (total)	1330-20-7	6.87E-02 e	8.49E-06 e	6.73e-03 a	1.75e+02 a

(continued)

Table B-1. (continued)

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 SCDM (USEPA, 1997b).
- b Calculated based on USEPA, 1987.
- c USEPA, 2000.
- d Calculated based on Lyman, Reehl, and Rosenblatt, 1990.
- e Calculated based on WATER9 (USEPA, 2001).
- f CHEMFATE (SRC, 1999).
- g ChemFinder.com (CambridgeSoft Corporation, 2001).
- h The Merck Index (Budavari, 1996).
- i HSDB (NLM, 2001).
- j Calculated based on USEPA, 2000.
- k USEPA, 1997a.

B.6 References for Attachment B

Budavari, S. (ed). 1996. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals*. 12th edition. Whitehouse Station, NJ: Merck and Co.

CambridgeSoft Corporation. 2001. ChemFinder.com database and internet searching. <http://chemfinder.cambridgesoft.com>. Accessed July 2001.

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1990. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds*. Washington, DC: American Chemical Society.

Syracuse Research Corporation (SRC). 1999. CHEMFATE Chemical Search, Environmental Science Center, Syracuse, NY. <http://esc.syrres.com/efdb/Chemfate.htm>. Accessed July 2001.

USEPA. 1987. *Process Coefficients and Models for Simulating Toxic Organics and Heavy Metals in Surface Waters*. Office of Research and Development. Washington, DC: U.S. Government Printing Office (GPO).

USEPA. 1997a. *Mercury Study Report to Congress. Volume IV: An Assessment of Exposure to Mercury in the United States*. EPA-452/R-97-006. Office of Air Quality Planning and Standards and Office of Research and Development. Washington, DC: GPO.

USEPA. 1997b. Superfund Chemical Data Matrix (SCDM). SCDMWIN 1.0 (SCDM Windows User's Version), Version 1. Office of Solid Waste and Emergency Response, Washington DC: GPO. <http://www.epa.gov/superfund/resources/scdm/index.htm>. Accessed July 2001.

USEPA. 2000. *Exposure and Human Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds, Part 1, Vol. 3*. Office of Research and Development, Washington, DC: GPO.

USEPA. 2001. WATER9. Office of Air Quality Planning and Standards, Research Triangle Park, NC. <http://www.epa.gov/ttn/chief/software/water/index.html>. Accessed July 2001.

USNLM (U.S. National Library of Medicine). 2001. Hazardous Substances Data Bank (HSDB). <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>. Accessed July 2001.

Attachment C

Human Health Benchmarks used in Developing the Revised Tier 1 Tool

Attachment C

Human Health Benchmarks used in the Revised Tier 1 Tool

Human health benchmarks for chronic oral and inhalation exposures are an important component of the Tier 1 tool. The U.S. Environmental Protection Agency (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 memorandum provides the toxicity benchmarks we used to develop the HBNs that we will use in developing the Tier 1 tool. Section C.1 describes the data sources and general hierarchy used to collect these benchmarks. Section C.2 provides the benchmarks along with discussions of individual human health benchmarks extracted from a variety of sources.

C.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 HEAST CSF for 2,3,7,8-TCDD to obtain CSFs for all other dioxins and furans (see Section C.2.4).

C.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 Tier 1 tool whenever IRIS benchmarks were available. IRIS is EPA's electronic database containing information on human health effects (USEPA, 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:

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

In this equation, 70 kg represents average body weight; 20 m³/d represents average inhalation rate; and 1000 μg/mg is a units conversion factor (USEPA, 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.

C.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 Tier 1 tool are described in Section C.2.5.

C.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 (USEPA, 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.

C.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.

C.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.

C.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 C.2.6 describes the specific values from these alternative EPA sources that were used in the Tier 1 tool.

C.2 Human Health Benchmarks used in the Tier 1 Tool

The chronic human health benchmarks used to calculate the health-based numbers (HBNs) in the Tier 1 tool are summarized in Table C-1, which provides the Chemical Abstract Service Registry Number (CASRN), constituent name, RfD (mg/kg-d), RfC (mg/m³), oral CSF (mg/kg-d⁻¹), inhalation URF [(μg/m³)⁻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 Tier 1 constituents, human health benchmarks were available from IRIS (USEPA, 2001a), Superfund Provisional Benchmarks, or HEAST (USEPA, 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 C-1. Human Health Benchmarks Used in the Tier 1 Tool

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	CSFo Ref	RfC		URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)		CSFi Ref
		(mg/kg-d)	RfD Ref			(mg/m3)	RfC Ref			(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									

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	RfC			URF (per ug/m3)	CSFi (per mg/kg-d)		
		(mg/kg-d)	RfD Ref		CSFo Ref	(mg/m3)	RfC Ref		URF Ref	mg/kg-d)	CSFi Ref
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
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				
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								

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo	RfC			URF (per	CSFi (per		
		(mg/kg-d)	RfD Ref	(per mg/kg-d)	CSFo Ref	(mg/m3)	RfC Ref	ug/m3)	URF Ref	mg/kg-d)	CSFi Ref
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
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				

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	RfC			URF (per ug/m3)	CSFi (per mg/kg-d)		
		(mg/kg-d)	RfD Ref		CSFo Ref	(mg/m3)	RfC Ref		URF Ref	mg/kg-d)	CSFi Ref
Dichloropropene, <i>trans</i> -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, <i>cis</i> -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 phthalate	131-11-3										
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
Dimethylbenzidine, 3,3'-	119-93-7			9.2E+00	H						
Dimethylphenol, 2,4-	105-67-9	2.0E-02	I								
Dimethylphenol, 3,4-	95-65-8	1.0E-03	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				

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	RfC		URF (per ug/m3)	CSFi (per mg/kg-d)		
		(mg/kg-d)	RfD Ref		CSFo Ref	(mg/m3)	RfC Ref	URF Ref	mg/kg-d	CSFi Ref
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			
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							
Fluorene	86-73-7	4.0E-02	I							
Fluoride	16984-48-8	6.0E-02	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							
Furan	110-00-9	1.0E-03	I							
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			1.5E+04	WHO98			3.3E+00	WHO98	1.5E+04 WHO98
Hexachlorodibenzofurans (HxCDFs)	55684-94-1			1.5E+04	WHO98			3.3E+00	WHO98	1.5E+04 WHO98

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
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				
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								
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

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD (mg/kg-d)	RfD Ref	CSFo (per mg/kg-d)	CSFo Ref	RfC (mg/m3)	RfC Ref	URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)	CSFi Ref
N-Nitrosomethylethylamine	10595-95-6			2.2E+01	I			6.3E-03	C99a	3.7E+00	C99a
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 pyrophosphoramidate	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			1.5E+05	WHO98			3.3E+01	WHO98	1.5E+05	WHO98
Pentachlorodibenzofurans (PeCDFs)	30402-15-4			7.5E+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
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								

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	RfC		URF (per ug/m3)	CSFi (per mg/kg-d)		
		(mg/kg-d)	RfD Ref		CSFo Ref	(mg/m3)	RfC Ref	URF Ref	mg/kg-d)	CSFi Ref
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	1.0E-09	A	1.5E+05	H			3.3E+01	H	1.5E+05 H

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	RfC			URF (per ug/m3)	CSFi (per mg/kg-d)		
		(mg/kg-d)	RfD Ref		CSFo Ref	(mg/m3)	RfC Ref		URF Ref	mg/kg-d)	CSFi Ref
Tetrachlorodibenzofuran, 2,3,7,8-(2,3,7,8-TCDF)	51207-31-9			1.5E+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
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				

Table C-1. Human Health Benchmarks Used in the Tier 1 Tool (continued)

Constituent Name	CASRN	RfD		CSFo (per mg/kg-d)	CSFo Ref	RfC		URF (per ug/m3)	URF Ref	CSFi (per mg/kg-d)		CSFi Ref
		(mg/kg-d)	RfD Ref			(mg/m3)	RfC Ref			mg/kg-d)		
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)					
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.

RfD = reference dose.

RfC = reference concentration.

CSFo = oral cancer slope factor.

CSFi = inhalation cancer slope factor.

URF = unit risk factor.

^a Sources:

A = ATSDR MRLs (ATSDR, 2001)

AC = developed for the Air Characteristic Study (USEPA, 1999g)

calc = calculated

C99a = CalEPA cancer potency factor (CalEPA, 1999a)

C99b = CalEPA chronic REL (CalEPA, 1999b) solv

C00 = CalEPA chronic REL (CalEPA, 2000)

HAD = Health Assessment Document (USEPA, 1986a, 1987)

H = HEAST (USEPA, 1997)

I = IRIS (USEPA, 2001a)

RQ = reportable quantity adjustments (USEPA, 1998d,e,f)

SF = Superfund Risk Issue Paper (USEPA, 1998a,b; 1999a,b,c,d,e,f; 2000, 2001b,c,d)

= 63 FR 64371-0402 (USEPA, 1998c)

surr = surrogate (source in parentheses; see section C.2.8)

TEF = toxicity equivalency factor (USEPA, 1993)

WHO98= World Health Organization (WHO) 1998 toxicity equivalency factor scheme (Van den Berg et al., 1998)

C.2.1 Benzene

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

C.2.2 Vinyl Chloride

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

C.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 will be used for the Tier 1 tool.

C.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 knowledge of a contaminant’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 Tier 1 tool.

²A 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 the Tier 1 Tool.

³A twofold increase to $8.8\text{E-}6$ per $\mu\text{g/m}^3$ for the inhalation URF, to account for continuous lifetime exposure from birth, was also recommended but was not used for the Tier 1 tool.

The dioxin-like congeners (and groups of congeners) included in the Tier 1 tool 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 C-2 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 C-2. TEFs Used for Dioxin and Furan Congeners

Constituent Name	TEF	CSFo (mkd) ⁻¹	CSFo Source	URF (µg/m ³) ⁻¹	URF Source	CSFi (mkd) ⁻¹	CSFi Source
Dioxins							
Pentachlorodibenzodioxins	1	1.5E+05	WHO 1998	3.3E+01	WHO 1998	1.5E+05	WHO 1998
2,3,7,8-TCDD	1	1.5E+5	EPA, 1997	3.3E+01	EPA, 1997	1.5E+5	EPA, 1997
Hexachlorodibenzodioxins	0.1	1.5E+4	WHO 1998	3.3E+00	WHO 1998	1.5E+4	WHO 1998
Furans							
Hexachlorodibenzofurans	0.1	1.5E+4	WHO 1998	3.3E+00	WHO 1998	1.5E+4	WHO 1998
Pentachlorodibenzofurans	0.5	7.5E+4	WHO 1998	1.7E+01	WHO 1998	7.5E+4	WHO 1998
2,3,7,8-TCDF	0.1	1.5E+4	WHO 1998	3.3E+00	WHO 1998	1.5E+4	WHO 1998

WHO 98 = TEFs presented in Van den Berg et al. (1998)

EPA, 1997 = HEAST (USEPA, 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.

C.2.5 Superfund Technical Support Center Provisional Benchmarks

Table C-3 lists the provisional human health benchmarks from the Superfund Technical Support Center that were used for some the Tier 1 constituents. A provisional subchronic RfC of 2.0E-2 mg/m³ was developed by the Superfund Technical Support Center (USEPA, 1999a) for carbon tetrachloride; a provisional chronic RfC of 7.0E-3 mg/m³ was derived from this value by applying an uncertainty factor of 3 to account for the use of a subchronic study.

Table C-3. Provisional Human Health Benchmarks Developed by the Superfund Technical Support Center

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

C.2.6 Benchmarks From Other EPA Sources

For some Tier 1 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/m³, and the provisional inhalation CSF of 2.0E-3 per mg/kg-d developed for

tetrachloroethylene by EPA in a Health Assessment Document (HAD) (USEPA, 1986a) were used.

- For trichloroethylene, provisional cancer benchmarks developed by EPA in a HAD (USEPA, 1987) were used and include the oral CSF of $1.1\text{E-}2$ per mg/kg-d, inhalation URF of $1.7\text{E-}6$ per $\mu\text{g/m}^3$, and inhalation CSF of $6.0\text{E-}3$ per mg/kg-d.
- A provisional RfD of $1.7\text{E-}5$ mg/kg-d and a provisional RfC of $2.0\text{E-}5$ mg/ m^3 were derived for cyclohexanol in the final listing rule for solvents (63 FR 64371) and were used (USEPA, 1998c).
- An acceptable daily intake (ADI) of $2.0\text{E-}03$ mg/kg-d from inhalation ($7.0\text{E-}3$ mg/ m^3) was identified for pyridine (USEPA, 1986b).
- EPA calculated an oral cancer potency factor of 293 per mg/kg-d for ethyl methanesulfonate in a reportable quantity adjustment evaluation (USEPA, 1998d).
- EPA calculated an oral cancer potency factor of 0.18 per mg/kg-d for safrole in a reportable quantity adjustment evaluation (USEPA, 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 (USEPA, 1998f).
- The cancer slope factor for dibenzo(a,h)anthracene was calculated using a TEF approach developed for polycyclic aromatic hydrocarbons (USEPA, 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 (USEPA, 2001a) value for benzo(a)pyrene: $7.3\text{E+}00$ (mg/kg-d)⁻¹.

C.2.7 Air Characteristic Study Provisional Benchmarks

Provisional inhalation health benchmarks were developed in the Air Characteristic Study (USEPA, 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 C-4 below. Additional details on the derivation of these inhalation benchmarks can be found in the *Revised Risk Assessment for the Air Characteristic Study* (USEPA, 1999g).

Table C-4. 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

C.2.8 Surrogate Health Benchmarks

For several Tier 1 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/m³. The oral CSF for 1,3-dichloropropene is 0.1 (mg/kg-d)⁻¹ and the inhalation URF is 4E-06 (µg/m³)⁻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 (6E-02 mg/kg-d) is based on soluble fluoride.
- 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.

C.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 (USEPA, 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 (USEPA, 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 (USEPA, 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..."(USEPA, 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" (USEPA, 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/m³) was used in Tier 1.

C.3 References

ATSDR. 2001. *Minimal Risk Levels (MRLs) for Hazardous Substances*.

<http://atsdr1.atsdr.cdc.gov:8080/mrls.html>

CalEPA. 1999a. *Air Toxics Hot Spots Program Risk Assessment Guidelines: Part II. Technical Support Document for Describing Available Cancer Potency Factors*. Office of Environmental Health Hazard Assessment, Berkeley, CA. Available online at <http://www.oehha.org/scientific/hasca2.htm>.

CalEPA. 1999b. *Air Toxics Hot Spots Program Risk Assessment Guidelines: Part III. Technical Support Document for the Determination of Noncancer Chronic Reference Exposure Levels*. SRP Draft. Office of Environmental Health Hazard Assessment, Berkeley, CA. Available online at <http://www.oehha.org/hotspots/RAGSII.html>.

CalEPA. 2000. *Air Toxics Hot Spots Program Risk Assessment Guidelines: Part III. Technical Support Document for the Determination of Noncancer Chronic Reference Exposure Levels*. Office of Environmental Health Hazard Assessment, Berkeley, CA. Available online (in 3 sections) at http://www.oehha.org/air/chronic_rels/22RELS2k.html, http://www.oehha.org/air/chronic_rels/42kChREL.html, http://www.oehha.org/air/chronic_rels/Jan2001ChREL.html.

USEPA. 1986a. *Addendum to the Health Assessment Document for Tetrachloroethylene (Perchloroethylene). Updated Carcinogenicity Assessment for Tetrachloroethylene (Perchloroethylene, PERC, PCE)*. External Review Draft. EPA/600/8-82-005FA. Office of Health and Environmental Assessment, Office of Research and Development, Washington DC.

USEPA. 1986b. *Health and Environmental Effects Profile for Pyridine*. EPA/600/x-86-168. Environmental Criteria and Assessment Office, Office of Research and Development, Cincinnati, OH.

USEPA. 1987. *Addendum to the Health Assessment Document for Trichloroethylene. Updated Carcinogenicity Assessment for Trichloroethylene*. External Review Draft. EPA/600/8-82-006FA. Office of Health and Environmental Assessment, Office of Research and Development, Washington DC.

USEPA. 1993. *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons*. Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH. EPA/600/R-93-089.

- USEPA. 1994. *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry*. EPA/600/8-90-066F. Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, Research Triangle Park, NC.
- USEPA. 1997. *Health Effects Assessment Summary Tables (HEAST)*. EPA-540-R-97-036. FY 1997 Update. Office of Solid Waste and Emergency Response, Washington, DC.
- USEPA. 1998a. *Risk Assessment Issue Paper for: Derivation of a Provisional Chronic RfC for Chlorobenzene (CASRN 108-90-7)*. 98-020/09-18-98. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1998b. *Risk Assessment Paper for: Evaluation of the Systemic Toxicity of Hexachlorobutadiene (CASRN 87-68-3) Resulting from Oral Exposure*. 98-009/07-17-98. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1998c. Hazardous waste management system; identification and listing of hazardous waste; solvents; final rule. *Federal Register* 63 FR 64371-402.
- USEPA. 1998d. Evaluation of the Potential Carcinogenicity of Ethyl Methanesulfonate (62-50-0) in Support of Reportable Quantity Adjustments Pursuant to CERLCA Section 102. Prepared by Carcinogen Assessment Group, Office of Health and Environmental Assessment, Washington, D.C.
- USEPA. 1998e. Evaluation of the Potential Carcinogenicity of Safrole (94-59-7) in Support of Reportable Quantity Adjustments Pursuant to CERLCA Section 102. Prepared by Carcinogen Assessment Group, Office of Health and Environmental Assessment, Washington, D.C.
- USEPA. 1998f. Evaluation of the Potential Carcinogenicity of Tris(2,3-dibromopropyl)phosphate (126-72-7) in Support of Reportable Quantity Adjustments Pursuant to CERLCA Section 102. Prepared by Carcinogen Assessment Group, Office of Health and Environmental Assessment, Washington, D.C.
- USEPA. 1998g. National primary drinking water regulations: disinfectants and disinfection byproducts notice of data availability; Proposed Rule. *Federal Register* 63 (61): 15673-15692. March 31.
- USEPA. 1998h. National primary drinking water regulations: disinfectants and disinfection byproducts; final rule. *Federal Register* 63 (241): 69390-69476. December 16.

- USEPA. 1999a. *Risk Assessment Paper for: The Derivation of a Provisional Subchronic RfC for Carbon Tetrachloride (CASRN 56-23-5)*. 98-026/6-14-99. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1999b. *Risk Assessment Issue Paper for: Evaluating the Carcinogenicity of Ethylbenzene (CASRN 100-41-4)*. 99-011/10-12-99. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1999c. *Risk Assessment Paper for: An Updated Systemic Toxicity Evaluation of n-Hexane (CASRN 110-54-3)*. 98-019/10-1-99. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1999d. *Risk Assessment Issue Paper for: Derivation of Provisional Oral Chronic RfD and Subchronic RfDs for 1,1,1-Trichloroethane (CASRN 71-55-6)*. 98-025/8-4-99. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1999e. *Risk Assessment Issue Paper for: Derivation of Provisional Chronic and Subchronic RfCs for 1,1,1-Trichloroethane (CASRN 71-55-6)*. 98-025/8-4-99. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1999f. *Risk Assessment Paper for: Derivation of the Systemic Toxicity of 1,2,3-Trichloropropane (CASRN 96-18-4)*. 98-014/8-13-99. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 1999g. *Revised Risk Assessment for the Air Characteristic Study*. EPA-530-R-99-019a. Volume 2. Office of Solid Waste, Washington, DC.
- USEPA. 2000. *Risk Assessment Paper for: Derivation of a Provisional RfD for 1,1,2,2-Tetrachloroethane (CASRN 79-34-5)*. 00-122/12-20-00. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 2001a. Integrated Risk Information System (IRIS). National Center for Environmental Assessment, Office of Research and Development, Washington, DC. Available online at <http://www.epa.gov/iris/>
- USEPA. 2001b. *Risk Assessment Paper for: Derivation of a Provisional RfD for Cobalt and Compounds (CASRN 7440-48-4)*. 00-122/3-16-01. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.
- USEPA. 2001c. *Risk Assessment Paper for: Derivation of a Provisional RfD for N-Nitrosodimethylamine (CASRN 62-75-9)*. 00-122/3-16-01. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.

USEPA. 2001d. *Risk Assessment Paper for: Derivation of a Provisional RfD for N-Nitrosodiphenylamine (CASRN 86-30-6)*. 00-122/3-16-01. National Center for Environmental Assessment. Superfund Technical Support Center, Cincinnati, OH.

Van den Berg, M., L. Birnbaum, A.T.C. Bosveld, et al. 1998. Toxic equivalency factors (TEFs) for PCBs, PCDDs, PCDFs for humans and wildlife. *Environmental Health Perspectives* 106:775-792.