Part 2: DEVELOPMENT OF PATHWAY-SPECIFIC SOIL SCREENING LEVELS

This part of the Technical Background Document describes the methods used to calculate SSLs for residential exposure pathways, along with their technical basis and limitations associated with their use. Simple, standardized equations have been developed for three common exposure pathways at Superfund sites:

- Ingestion of soil (Section 2.2)
- Inhalation of volatiles and fugitive dust (Section 2.4)
- Ingestion of contaminated ground water caused by migration of contaminants through soil to an underlying potable aquifer (Section 2.5).

The equations were developed under the following constraints:

- They should be consistent with current Superfund risk assessment methodologies and guidance.
- To be appropriate for early-stage application, they should be simple and easy to apply.
- They should allow the use of site-specific data where they are readily available or can be easily obtained.
- The process of developing and applying SSLs should generate information that can be used and built upon as a site evaluation progresses.

The equations for the inhalation and migration to ground water pathways include easily obtained site-specific input parameters. Conservative default values have been developed for use where site-specific data are not available. Generic SSLs, calculated for 110 chemicals using these default values, are presented in Appendix A. The generic SSLs are conservative, since the default values are designed to be protective at most sites across the country.

The inhalation and migration to ground water pathway equations assume an infinite source. As pointed out by several commenters to the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h), SSLs developed using these models may violate mass-balance for certain contaminants and site conditions (e.g., small sources). To address this concern, EPA has incorporated simple mass-limit models for these pathways assuming that the entire volume of contamination either volatilizes or leaches over the duration of exposure and that the level of contaminant at the receptor does not exceed the health-based limit (Section 2.6). **Because they require a site-specific estimate of source depth, these models cannot be used to calculate generic SSLs.**

Dermal adsorption, consumption of garden vegetables grown in contaminated soil, and migration of volatiles into basements also may contribute significantly to the risk to human health from exposure to soil contaminants in a residential setting. These pathways have been incorporated into the Soil Screening Guidance to the greatest extent practical.

Although methods for quantifying dermal exposures are available, their use for calculating SSLs is limited by the amount of data available on dermal absorption of specific chemicals (Section 2.3). Screening equations have been developed to estimate human exposure from the uptake of soil contaminants by garden plants (Section 2.7). As with dermal absorption, the number of chemicals for which adequate empirical data on plant uptake are limited. An approach to address migration of volatiles into basements is presented in Section 2.8, and limitations of the approach are discussed.

Section 2.1 describes the human health basis of the Soil Screening Guidance and provides the human toxicity and health benchmarks necessary to calculate SSLs. The selection and development of the chemical properties required to calculate SSLs are described in Part 5 of this document.

2.1 Human Health Basis

Table 1 lists the regulatory and human health benchmarks necessary to calculate SSLs for 110 chemicals including:

- Ingestion SSLs: oral cancer slope factors (SF_o) and noncancer reference doses (RfDs)
- Inhalation SSLs: inhalation unit risk factors (URFs) and reference concentrations (RfCs)
- Migration to ground water SSLs: drinking water standards (MCLGs and MCLs) and drinking water health-based levels (HBLs).

The human health benchmarks in Table 1 were obtained from IRIS (U.S. EPA, 1995b) or HEAST (U.S. EPA, 1995d) unless otherwise indicated. MCLGs and MCLs were obtained from U.S. EPA (1995a). Each of these references is updated regularly. **Prior to calculating SSLs, the values in Table 1 should be checked against the most recent version of these sources to ensure that they are up-to-date.**

2.1.1 Additive Risk. For soil ingestion and inhalation of volatiles and fugitive dusts, SSLs correspond to a 10^{-6} risk level for carcinogens and a hazard quotient of 1 for noncarcinogens. For carcinogens, EPA believes that setting a 10^{-6} risk level for individual chemicals and pathways generally will lead to cumulative risks within the 10^{-4} to 10^{-6} range for the combinations of chemicals typically found at Superfund sites.

Whereas the carcinogenic risks of multiple chemicals are simply added together, the issue of additive risk is much more complex for noncarcinogens because of the theory that a threshold exists for noncancer effects. This threshold level, below which adverse effects are not expected to occur, is the basis for EPA's RfD and RfC. Since adverse effects are not expected to occur at the RfD or RfC and the SSLs were derived by setting the potential exposure dose equal to the RfD or RfC (i.e., an HQ equal to 1), it is difficult to address the risk of exposure to multiple chemicals at levels where the individual chemicals alone would not be expected to cause any harmful effect. However, problems may arise when multiple chemicals produce related toxic effects.

EPA believes, and the Science Advisory Board (SAB) agrees (U.S. EPA, 1993e), that HQs should be added only for those chemicals with the same toxic endpoint and/or mechanism of action.

Table 1. Regulatory and Human Health Benchmarks Used for SSL Development

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor $(mg/kg\text{-}d)^{-1}$			Unit Risk Factor $(\mu g/m^3)^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	Chemical Name	MCLG (PMCLG)	Ref. [a]	MCL (PMCL)	Ref. [a]	HBL [b]	Basis	Carc. Class [c]	SF_o	Ref. [a]	Carc. Class [c]	URF	Ref. [a]	RfD	Ref. [a]	RfC	Ref. [a]
83-32-9	Acenaphthene					2E+00	RfD							6.0E-02	1		
67-64-1	Acetone (2-Propanone)					4E+00	RfD	D			D			1.0E-01	1		
309-00-2	Aldrin					5E-06	SF_o	B2	1.7E+01	1	B2	4.9E-03	1	3.0E-05	1		
120-12-7	Anthracene					1E+01	RfD	D			D			3.0E-01	1		
7440-36-0	Antimony	6.0E-03	3	6.0E-03	3									4.0E-04	1		
7440-38-2	Arsenic			5.0E-02	3			A	1.5E+00	1	A	4.3E-03	1	3.0E-04	1		
7440-39-3	Barium	2.0E+00	3	2.0E+00	3									7.0E-02	1	5.0E-04	2
56-55-3	Benz(*a*)anthracene					1E-04	SF_o	B2	7.3E-01	4	B2						
71-43-2	Benzene			5.0E-03	3			A	2.9E-02	1	A	8.3E-06	1				
205-99-2	Benzo(*b*)fluoranthene					1E-04	SF_o	B2	7.3E-01	4	B2						
207-08-9	Benzo(*k*)fluoranthene					1E-03	SF_o	B2	7.3E-02	4	B2						
65-85-0	Benzoic acid					1E+02	RfD							4.0E+00	1		
50-32-8	Benzo(*a*)pyrene			2.0E-04	3			B2	7.3E+00	1	B2						
7440-41-7	Beryllium	4.0E-03	3	4.0E-03	3			B2	4.3E+00	1	B2	2.4E-03	1	5.0E-03	1		
111-44-4	Bis(2-chloroethyl)ether					8E-05	SF_o	B2	1.1E+00	1	B2	3.3E-04	1				
117-81-7	Bis(2-ethylhexyl)phthalate			6.0E-03	3			B2	1.4E-02	1	B2			2.0E-02	1		
75-27-4	Bromodichloromethane			1.0E-01 *	3			B2	6.2E-02	1	B2			2.0E-02	1		
75-25-2	Bromoform (tribromomethane)			1.0E-01 *	3			B2	7.9E-03	1	B2	1.1E-06	1	2.0E-02	1		
71-36-3	Butanol					4E+00	RfD	D			D			1.0E-01	1		
85-68-7	Butyl benzyl phthalate					7E+00	RfD	C			C			2.0E-01	1		
7440-43-9	Cadmium	5.0E-03	3	5.0E-03	3						B1	1.8E-03	1	1.0E-03**	1		
86-74-8	Carbazole					4E-03	SF_o	B2	2.0E-02	2							
75-15-0	Carbon disulfide					4E+00	RfD							1.0E-01	1	7.0E-01	1
56-23-5	Carbon tetrachloride			5.0E-03	3			B2	1.3E-01	1	B2	1.5E-05	1	7.0E-04	1		
57-74-9	Chlordane			2.0E-03	3			B2	1.3E+00	1	B2	3.7E-04	1	6.0E-05	1		
106-47-8	*p* -Chloroaniline					1E-01	RfD							4.0E-03	1		
108-90-7	Chlorobenzene	1.0E-01	3	1.0E-01	3			D			D			2.0E-02	1	2.0E-02	2
124-48-1	Chlorodibromomethane	6.0E-02	3	1.0E-01 *	3			C	8.4E-02	1	C			2.0E-02	1		
67-66-3	Chloroform			1.0E-01 *	3			B2	6.1E-03	1	B2	2.3E-05	1	1.0E-02	1		
95-57-8	2-Chlorophenol					2E-01	RfD							5.0E-03	1		

* Proposed MCL = 0.08 mg/L, *Drinking Water Regulations and Health Advisories* , U.S. EPA (1995).

** Cadmium RfD is based on dietary exposure.

Table 1 (continued)

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor (mg/kg-d)$^{-1}$			Unit Risk Factor (μg/m^3)$^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	Chemical Name	MCLG (PMCLG)	Ref. [a]	MCL (PMCL)	Ref. [a]	HBL [b]	Basis	Carc. Class [c]	SF_o	Ref. [a]	Carc. Class [c]	URF	Ref. [a]	RfD	Ref. [a]	RfC	Ref. [a]
7440-47-3	Chromium	1.0E-01	3	1.0E-01	3			A			A	1.2E-02	1	5.0E-03	1		
16065-83-1	Chromium (III)					4E+01	RfD							1.0E+00	1		
18540-29-9	Chromium (VI)			1.0E-01	3 *			A			A	1.2E-02	1	5.0E-03	1		
218-01-9	Chrysene					1E-02	SF_o	B2	7.3E-03	4							
57-12-5	Cyanide (amenable)	(2.0E-01)	3	(2.0E-01)	3			D			D			2.0E-02	1		
72-54-8	DDD					4E-04	SF_o	B2	2.4E-01	1	B2						
72-55-9	DDE					3E-04	SF_o	B2	3.4E-01	1	B2						
50-29-3	DDT					3E-04	SF_o	B2	3.4E-01	1	B2	9.7E-05	1	5.0E-04	1		
53-70-3	Dibenz(*a,h*)anthracene					1E-05	SF_o	B2	7.3E+00	4	B2						
84-74-2	Di-*n* -butyl phthalate					4E+00	RfD	D			D			1.0E-01	1		
95-50-1	1,2-Dichlorobenzene	6.0E-01	3	6.0E-01	3			D			D			9.0E-02	1	2.0E-01	2
106-46-7	1,4-Dichlorobenzene	7.5E-02	3	7.5E-02	3			B2	2.4E-02	2	B2					8.0E-01	1
91-94-1	3,3-Dichlorobenzidine					2E-04	SF_o	B2	4.5E-01	1	B2						
75-34-3	1,1-Dichloroethane					4E+00	RfD	C			C			1.0E-01	7	5.0E-01	2
107-06-2	1,2-Dichloroethane			5.0E-03	3			B2	9.1E-02	1	B2	2.6E-05	1				
75-35-4	1,1-Dichloroethylene	7.0E-03	3	7.0E-03	3			C	6.0E-01	1	C	5.0E-05	1	9.0E-03	1		
156-59-2	*cis* -1,2-Dichloroethylene	7.0E-02	3	7.0E-02	3			D			D			1.0E-02	2		
156-60-5	*trans* -1,2-Dichloroethylene	1.0E-01	3	1.0E-01	3									2.0E-02	1		
120-83-2	2,4-Dichlorophenol					1E-01	RfD							3.0E-03	1		
78-87-5	1,2-Dichloropropane			5.0E-03	3			B2	6.8E-02	2	B2					4.0E-03	1
542-75-6	1,3-Dichloropropene					5E-04	SF_o	B2	1.8E-01	2	B2	3.7E-05	2	3.0E-04	1	2.0E-02	1
60-57-1	Dieldrin					5E-06	SF_o	B2	1.6E+01	1	B2	4.6E-03	1	5.0E-05	1		
84-66-2	Diethylphthalate					3E+01	RfD	D			D			8.0E-01	1		
105-67-9	2,4-Dimethylphenol					7E-01	RfD							2.0E-02	1		
51-28-5	2,4-Dinitrophenol					4E-02	RfD							2.0E-03	1		
121-14-2	2,4-Dinitrotoluene**					1E-04	SF_o	B2	6.8E-01	1				2.0E-03	1		
606-20-2	2,6-Dinitrotoluene**					1E-04	SF_o	B2	6.8E-01	1				1.0E-03	2		
117-84-0	Di-*n* -octyl phthalate					7E-01	RfD							2.0E-02	2		
115-29-7	Endosulfan					2E-01	RfD							6.0E-03	2		
72-20-8	Endrin	2.0E-03	3	2.0E-03	3			D			D			3.0E-04	1		

* MCL for total chromium is based on Cr (VI) toxicity.

** Cancer Slope Factor is for 2,4-, 2,6-Dinitrotoluene mixture.

Table 1 (continued)

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor $(mg/kg\text{-}d)^{-1}$			Unit Risk Factor $(\mu g/m^3)^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	**Chemical Name**	**MCLG (PMCLG)**	**Ref.** [a]	**MCL (PMCL)**	**Ref.** [a]	**HBL** [b]	**Basis**	**Carc. Class** [c]	**SF_o**	**Ref.** [a]	**Carc. Class** [c]	**URF**	**Ref.** [a]	**RfD**	**Ref.** [a]	**RfC**	**Ref.** [a]
100-41-4	Ethylbenzene	7.0E-01	3	7.0E-01	3			D			D			1.0E-01	1	1.0E+00	1
206-44-0	Fluoranthene					1E+00	RfD	D			D			4.0E-02	1		
86-73-7	Fluorene					1E+00	RfD	D						4.0E-02	1		
76-44-8	Heptachlor			4.0E-04	3			B2	4.5E+00	1	B2	1.3E-03	1	5.0E-04	1		
1024-57-3	Heptachlor epoxide			2.0E-04	3			B2	9.1E+00	1	B2	2.6E-03	1	1.3E-05	1		
118-74-1	Hexachlorobenzene			1.0E-03	3			B2	1.6E+00	1	B2	4.6E-04	1	8.0E-04	1		
87-68-3	Hexachloro-1,3-butadiene	1.0E-03	3			1E-03	SF_o	C	7.8E-02	1	C	2.2E-05	1	2.0E-04	2		
319-84-6	α-HCH (α-BHC)					1E-05	SF_o	B2	6.3E+00	1	B2	1.8E-03	1				
319-85-7	β-HCH (β-BHC)					5E-05	SF_o	C	1.8E+00	1	C	5.3E-04	1				
58-89-9	γ-HCH (Lindane)	2.0E-04	3	2.0E-04	3			B2	1.3E+00	2	C			3.0E-04	1		
77-47-4	Hexachlorocyclopentadiene	5.0E-02	3	5.0E-02	3			D			D			7.0E-03	1	7.0E-05	2
67-72-1	Hexachloroethane					6E-03	SF_o	C	1.4E-02	1	C	4.0E-06	1	1.0E-03	1		
193-39-5	Indeno(1,2,3-*cd*)pyrene					1E-04	SF_o	B2	7.3E-01	4	B2						
78-59-1	Isophorone					9E-02	SF_o	C	9.5E-04	1	C			2.0E-01	1		
7439-97-6	Mercury	2.0E-03	3	2.0E-03	3			D			D			3.0E-04	2	3.0E-04	2
72-43-5	Methoxychlor	4.0E-02	3	4.0E-02	3			D			D			5.0E-03	1		
74-83-9	Methyl bromide					5E-02	RfD	D			D			1.4E-03	1	5.0E-03	1
75-09-2	Methylene chloride			5.0E-03	3			B2	7.5E-03	1	B2	4.7E-07	1	6.0E-02	1	3.0E+00	2
95-48-7	2-Methylphenol (*o* -cresol)					2E+00	RfD	C			C			5.0E-02	1		
91-20-3	Naphthalene					1E+00	RfD	D			D			4.0E-02	6		
7440-02-0	Nickel					1E-01	HA *	A			A	2.4E-04	1	2.0E-02	1		
98-95-3	Nitrobenzene					2E-02	RfD	D			D			5.0E-04	1	2.0E-03	2
86-30-6	*N* -Nitrosodiphenylamine					2E-02	SF_o	B2	4.9E-03	1	B2						
621-64-7	*N* -Nitrosodi-*n* -propylamine					1E-05	SF_o	B2	7.0E+00	1	B2						
87-86-5	Pentachlorophenol			1.0E-03	3			B2	1.2E-01	1	B2			3.0E-02	1		
108-95-2	Phenol					2E+01	RfD	D			D			6.0E-01	1		
129-00-0	Pyrene					1E+00	RfD	D			D			3.0E-02	1		
7782-49-2	Selenium	5.0E-02	3	5.0E-02	3			D			D			5.0E-03	1		
7440-22-4	Silver					2E-01	RfD	D			D			5.0E-03	1		
100-42-5	Styrene	1.0E-01	3	1.0E-01	3									2.0E-01	1	1.0E+00	1
79-34-5	1,1,2,2-Tetrachloroethane					4E-04	SF_o	C	2.0E-01	1	C	5.8E-05	1				

* Health advisory for nickel (MCL is currently remanded); EPA Office of Science and Technology, 7/10/95.

Table 1 (continued)

		Maximum Contaminant Level Goal (mg/L)		Maximum Contaminant Level (mg/L)		Water Health Based Limits (mg/L)		Cancer Slope Factor $(mg/kg\text{-}d)^{-1}$			Unit Risk Factor $(\mu g/m^3)^{-1}$			Reference Dose (mg/kg-d)		Reference Concentration (mg/m^3)	
CAS Number	Chemical Name	MCLG (PMCLG)	Ref. [a]	MCL (PMCL)	Ref. [a]	HBL [b]	Basis	Carc. Class [c]	SF_o	Ref. [a]	Carc. Class [c]	URF	Ref. [a]	RfD	Ref. [a]	RfC	Ref. [a]
127-18-4	Tetrachloroethylene			5.0E-03	3				5.2E-02	5		5.8E-07	5	1.0E-02	1		
7440-28-0	Thallium	5.0E-04	3	2.0E-03	3												
108-88-3	Toluene	1.0E+00	3	1.0E+00	3			D			D			2.0E-01	1	4.0E-01	1
8001-35-2	Toxaphene			3.0E-03	3			B2	1.1E+00	1	B2	3.2E-04	1				
120-82-1	1,2,4-Trichlorobenzene	7.0E-02	3	7.0E-02	3			D			D			1.0E-02	1	2.0E-01	2
71-55-6	1,1,1-Trichloroethane	2.0E-01	3	2.0E-01	3			D			D					1.0E+00	5
79-00-5	1,1,2-Trichloroethane	3.0E-03	3	5.0E-03	3			C	5.7E-02	1	C	1.6E-05	1	4.0E-03	1		
79-01-6	Trichloroethylene	zero	3	5.0E-03	3				1.1E-02	5		1.7E-06	5				
95-95-4	2,4,5-Trichlorophenol					4E+00	RfD							1.0E-01	1		
88-06-2	2,4,6-Trichlorophenol					8E-03	SF_o	B2	1.1E-02	1	B2	3.1E-06	1				
7440-62-2	Vanadium					3E-01	RfD							7.0E-03	2		
108-05-4	Vinyl acetate					4E+01	RfD							1.0E+00	1	2.0E-01	1
75-01-4	Vinyl chloride (chloroethene)			2.0E-03	3			A	1.9E+00	2	A	8.4E-05	2				
108-38-3	*m* -Xylene	1.0E+01	3 *	1.0E+01	3 *			D			D			2.0E+00	2		
95-47-6	*o* -Xylene	1.0E+01	3 *	1.0E+01	3 *			D			D			2.0E+00	2		
106-42-3	*p* -Xylene	1.0E+01	3 *	1.0E+01	3 *			D			D			2.0E+00	1 **		
7440-66-6	Zinc					1E+01	RfD	D			D			3.0E-01	1		

* MCL for total xylenes [1330-20-7] is 10 mg/L.

** RfD for total xylenes is 2 mg/kg-day.

[a] References:
1 = IRIS, U.S. EPA (1995b)
2 = HEAST, U.S. EPA (1995d)
3 = U.S. EPA (1995a)
4 = OHEA, U.S. EPA (1993c)
5 = Interim toxicity criteria provided by Superfund Health Risk Techincal Support Center, Environmental Criteria Assessment Office (ECAO), Cincinnati, OH (1994)
6 = ECAO, U.S. EPA (1994g)
7 = ECAO, U.S. EPA (1994f)

[b] Health Based Limits calculated for 30-year exposure duration, 10^{-6} risk or hazard quotient = 1.

[c] Categorization of overall weight of evidence for human carcinogenicity:
Group A: human carcinogen
Group B: probable human carcinogen
B1: limited evidence from epidemiologic studies
B2: "sufficient" evidence from animal studies and "inadequate" evidence or "no data" from epidemiologic studies
Group C: possible human carcinogen
Group D: not classifiable as to health carcinogenicity
Group E: evidence of noncarcinogenicity for humans

Additivity of the SSLs for noncarcinogenic chemicals is further complicated by the fact that not all SSLs are based on toxicity. Some SSLs are determined instead by a "ceiling limit" concentration (C_{sat}) above which these chemicals may occur as nonaqueous phase liquids (NAPLs) in soil (see Section 2.4.4). Therefore, the potential for additive effects must be carefully evaluated at every site by considering the total Hazard Index (HI) for chemicals with RfDs or RfCs based on the same endpoint of toxicity (i.e., has the same critical effect as defined by the Reference Dose Methodology), excluding chemicals with SSLs based on C_{sat}. Table 2 lists several SSL chemicals with RfDs/RfCs, grouping those chemicals whose RfDs or RfCs are based on toxic effects in the same target organ or system. However, this list is limited, and a toxicologist should be consulted prior to addressing additive risks at a specific site.

2.1.2 Apportionment and Fractionation. EPA also has evaluated the SSLs for noncarcinogens in light of two related issues: apportionment and fractionation. **Apportionment** is typically used as the percentage of a regulatory health-based level that is allocated to the source/pathway being regulated (e.g., 20 percent of the RfD for the migration to ground water pathway). Apportioning risk assumes that the applied dose from the source, in this case contaminated soils, is only one portion of the total applied dose received by the receptor. In the Superfund program, EPA has traditionally focused on quantifying exposures to a receptor that are clearly site-related and has not included exposures from other sources such as commercially available household products or workplace exposures. Depending on the assumptions concerning other source contributions, apportionment among pathways and sources at a site may result in **more conservative** regulatory levels (e.g., levels that are below an HQ of 1). Depending on site conditions, this may be appropriate on a site-specific basis.

In contrast to apportionment, **fractionation** of risk may lead to **less conservative** regulatory levels because it assumes that some fraction of the contaminant does not reach the receptor due to partitioning into another medium. For example, if only one-fifth of the source is assumed to be available to the ground water pathway, and the remaining four-fifths is assumed to be released to air or remain in the soil, an SSL for the migration to ground water pathway could be set at five times the HQ of 1 due to the decrease in exposure (since only one-fifth of the possible contaminant is available to the pathway). However, the data collected to apply SSLs generally will not support the finite source models necessary for partitioning contaminants between pathways.

2.1.3 Acute Exposures. The exposure assumptions used to develop SSLs are representative of a chronic exposure scenario and do not account for situations where high-level exposures may lead to acute toxicity. For example, in some cases, children may ingest large amounts of soil (e.g., 3 to 5 grams) in a single event. This behavior, known as pica, may result in relatively high short-term exposures to contaminants in soils. Such exposures may be of concern for contaminants that primarily exhibit acute health effects. Review of clinical reports on contaminants addressed in this guidance suggests that acute effects of **cyanide** and **phenol** may be of concern in children exhibiting pica behavior. If soils containing cyanide and phenol are present at a site, the protectiveness of the chronic ingestion SSLs for these chemicals should be reconsidered.

Although the Soil Screening Guidance instructs site managers to consider the potential for acute exposures on a site-specific basis, there are two major impediments to developing **acute** SSLs. First, although data are available on chronic exposures (i.e., RfDs, RfCs, cancer slope factors), there is a paucity of data relating the potential for acute effects for most Superfund chemicals. Specifically, there is no scale to evaluate the severity of acute effects (e.g., eye irritation vs. dermatitis), no consensus on how to incorporate the body's recovery mechanisms following acute exposures, and no toxicity benchmarks to apply for short-term exposures (e.g., a 7-day RfD for a critical endpoint).

Table 2. SSL Chemicals with Noncarcinogenic Effects on Specific Target Organ/System

Target Organ/System	Effect
Kidney	
Acetone	Increased weight; nephrotoxicity
1,1-Dichloroethane	Kidney damage
Cadmium	Significant proteinuria
Chlorobenzene	Kidney effects
Di-*n*-octyl phthalate	Kidney effects
Endosulfan	Glomerulonephrosis
Ethylbenzene	Kidney toxicity
Fluoranthene	Nephropathy
Nitrobenzene	Renal and adrenal lesions
Pyrene	Kidney effects
Toluene	Changes in kidney weights
2,4,5-Trichlorophenol	Pathology
Vinyl acetate	Altered kidney weight
Liver	
Acenaphthene	Hepatotoxicity
Acetone	Increased weight
Butyl benzyl phthalate	Increased liver-to-body weight and liver-to-brain weight ratios
Chlorobenzene	Histopathology
Di-*n*-octyl phthalate	Increased weight; increased SGOT and SGPT activity
Endrin	Mild histological lesions in liver
Flouranthene	Increased liver weight
Nitrobenzene	Lesions
Styrene	Liver effects
Toluene	Changes in liver weights
2,4,5-Trichlorophenol	Pathology
Central Nervous System	
Butanol	Hypoactivity and ataxia
Cyanide (amenable)	Weight loss, myelin degeneration
2,4 Dimethylphenol	Prostatration and ataxia
Endrin	Occasional convulsions
2-Methylphenol	Neurotoxicity
Mercury	Hand tremor, memory disturbances
Styrene	Neurotoxicity
Xylenes	Hyperactivity
Adrenal Gland	
Nitrobenzene	Adrenal lesions
1,2,4-Trichlorobenzene	Increased adrenal weights; vacuolization in cortex

Table 2: (continued)

Target Organ/System	Effect
Circulatory System	
Antimony	Altered blood chemistry and myocardial effects
Barium	Increased blood pressure
trans-1,2-Dichloroethene	Increased alkaline phosphatase level
cis-1,2-Dichloroethylene	Decreased hematocrit and hemoglobin
2,4-Dimethylphenol	Altered blood chemistry
Fluoranthene	Hematologic changes
Fluorene	Decreased RBC and hemoglobin
Nitrobenzene	Hematologic changes
Styrene	Red blood cell effects
Zinc	Decrease in erythrocyte superoxide dismutase (ESOD)
Reproductive System	
Barium	Fetotoxicity
Carbon disulfide	Fetal toxicity and malformations
2-Chlorophenol	Reproductive effects
Methoxychlor	Excessive loss of litters
Phenol	Reduced fetal body weight in rats
Respiratory System	
1,2-Dichloropropane	Hyperplasia of the nasal mucosa
Hexachlorocyclopentadiene	Squamous metaplasia
Methyl bromide	Lesions on the olfactory epithelium of the nasal cavity
Vinyl acetate	Nasal epithelial lesions
Gastrointestinal System	
Hexachlorocyclopentadiene	Stomach lesions
Methyl bromide	Epithelial hyperplasia of the forestomach
Immune System	
2,4-Dichlorophenol	Altered immune function
p-Chloroaniline	Nonneoplastic lesions of splenic capsule

Source: U.S. EPA, 1995b, U.S. EPA, 1995d.

Second, the inclusion of acute SSLs would require the development of acute exposure scenarios that would be acceptable and applicable nationally. Simply put, the methodology and data necessary to address acute exposures in a standard manner analogous to that for chronic exposures have not been developed.

2.1.4 Route-to-Route Extrapolation. For a number of the contaminants commonly found at Superfund sites, inhalation benchmarks for toxicity are not available from IRIS or HEAST (see Table 1). Given that many of these chemicals exhibit systemic toxicity, EPA recognizes that the lack of such benchmarks could result in an underestimation of risk from contaminants in soil through the inhalation pathway. As pointed out by commenters to the December 1994 draft Soil Screening Guidance, ingestion SSLs tend to be higher than inhalation SSLs for most volatile chemicals with both inhalation and ingestion benchmarks. This suggests that ingestion SSLs may not be adequately protective for inhalation exposure to chemicals without inhalation benchmarks.

However, with the exception of vinyl chloride (which is gaseous at ambient temperatures), migration to ground water SSLs are significantly lower than inhalation SSLs for volatile organic chemicals (see the generic SSLs presented in Appendix A). Thus, at sites where ground water is of concern, migration to ground water SSLs generally will be protective from the standpoint of inhalation risk. However, if the ground water pathway is not of concern at a site, the use of SSLs for soil ingestion may not be adequately protective for the inhalation pathway.

To address this concern, OERR evaluated potential approaches for deriving inhalation benchmarks using route-to-route extrapolation from oral benchmarks (e.g., RfC_{inh} from RfD_{oral}). EPA evaluated a number of issues concerning route-to-route extrapolation, including: the potential reactivity of airborne toxicants (e.g., portal-of-entry effects), the pharmacokinetic behavior of toxicants for different routes of exposure (e.g., absorption by the gut versus absorption by the lung), and the significance of physicochemical properties in determining dose (e.g., vapor pressure, solubility). During this process, OERR consulted with staff in the EPA Office of Research and Development (ORD) to identify the most appropriate techniques for route-to-route extrapolation. Appendix B describes this analysis and its results.

As part of this analysis, inhalation benchmarks were derived using simple route-to-route extrapolation for 50 contaminants lacking inhalation benchmarks. A review of SSLs calculated from these extrapolated benchmarks indicated that for 36 of the 50 contaminants, inhalation SSLs exceed the soil saturation concentration (C_{sat}), often by several orders of magnitude. Because maximum volatile emissions occur at C_{sat} (see Section 2.4.4), these 36 contaminants are not likely to pose significant risks through the inhalation pathway at any soil concentration and the lack of inhalation benchmarks is not likely to underestimate risks. All of the 14 remaining contaminants with extrapolated inhalation SSLs below C_{sat} have inhalation SSLs above generic SSLs for the migration to ground water pathway (dilution attenuation factor [DAF] of 20). This suggests that migration to ground water SSLs will be adequately protective of volatile inhalation risks at sites where ground water is of concern.

At sites where ground water is not of concern (e.g., where ground water beneath or adjacent to the site is not a potential source of drinking water), the Appendix B analysis suggests that for certain contaminants, ingestion SSLs may not be protective of inhalation risks for contaminants lacking inhalation benchmarks. The analysis indicates that the extrapolated inhalation SSL values are below SSL values based on direct ingestion for the following chemicals: acetone, bromodichloromethane, chlorodibromomethane, *cis*-1,2-dichloroethylene, and *trans*-1,2-dichloroethylene. This supports the **possibility** that the SSLs based on direct ingestion for the listed chemicals may not be adequately protective of inhalation exposures. However, because this analysis is based on simplified route-to-route extrapolation methods, a more rigorous evaluation of route-to-route extrapolation methods may be warranted, especially at sites where ground water is not of concern.

Based on these results, EPA reached the following conclusions regarding the route-to-route extrapolation of inhalation benchmarks for the development of inhalation SSLs. First, it is reasonable to assume that, for some volatile contaminants, the lack of inhalation benchmarks may underestimate risks due to inhalation of volatile contaminants at a site. However, the analysis in Appendix B suggests that this issue is only of concern for sites where the exposure potential for the inhalation pathway approaches that for ingestion of ground water or at sites where the migration to ground water pathway is not of concern.

Second, the **extrapolated** inhalation SSL values are not intended to be used as generic SSLs for site investigations; the **extrapolated** inhalation SSLs are useful in determining the potential for inhalation risks but should not be misused as SSLs. The extrapolated inhalation benchmarks, used to calculate extrapolated inhalation SSLs, simply provide an estimate of the air concentration ($\mu g/m^3$)

required to produce an inhaled dose equivalent to the dose received via oral administration, and lack the scientific rigor required by EPA for route-to-route extrapolation. Route-to-route extrapolation methods must account for a relationship between physicochemical properties, absorption and distribution of toxicants, the significance of portal-of-entry effects, and the potential differences in metabolic pathways associated with the intensity and duration of inhalation exposures. However, methods required to develop sufficiently rigorous inhalation benchmarks have only recently been developed by the ORD. EPA's ORD has made available a guidance document that addresses many of the issues critical to the development of inhalation benchmarks. The document, entitled *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry* (U.S. EPA, 1994d), presents methods for applying inhalation dosimetry to derive inhalation reference concentrations and represents the current state-of-the-science at EPA with respect to inhalation benchmark development. The fundamentals of inhalation dosimetry are presented with respect to the toxicokinetic behavior of contaminants and the physicochemical properties of chemical contaminants.

Thus, at sites where the migration to ground water pathway is not of concern and a site manager determines that the inhalation pathway may be significant for contaminants lacking inhalation benchmarks, route-to-route extrapolation may be performed using EPA-approved methods on a case-by-case basis. Chemical-specific route-to-route extrapolations should be accompanied by a complete discussion of the data, underlying assumptions, and uncertainties identified in the extrapolation process. Extrapolation methods should be consistent with the EPA guidance presented in *Methods for Derivation of Inhalation Reference Concentrations and Applications of Inhalation Dosimetry* (U.S. EPA, 1994d). If a route-to-route extrapolation is found not to be appropriate based on the ORD guidance, the information on extrapolated SSLs may be included as part of the uncertainty analysis of the baseline risk assessment for the site.

2.2 Direct Ingestion

Calculation of SSLs for direct ingestion of soil is based on the methodology presented for residential land use in RAGS HHEM, Part B (U.S. EPA, 1991b). Briefly, this methodology backcalculates a soil concentration level from a target risk (for carcinogens) or hazard quotient (for noncarcinogens). A number of studies have shown that inadvertent ingestion of soil is common among children 6 years old and younger (Calabrese et al., 1989; Davis et al., 1990; Van Wijnen et al., 1990). Therefore, the approach uses an age-adjusted soil ingestion factor that takes into account the difference in daily soil ingestion rates, body weights, and exposure duration for children from 1 to 6 years old and others from 7 to 31 years old. The higher intake rate of soil by children and their lower body weights lead to a lower, or more conservative, risk-based concentration compared to an adult-only assumption. RAGS HHEM, Part B uses this age-adjusted approach for both noncarcinogens and carcinogens.

For noncarcinogens, the definition of an RfD has led to debates concerning the comparison of less-than-lifetime estimates of exposure to the RfD. Specifically, it is often asked whether the comparison of a 6-year exposure, estimated for children via soil ingestion, to the chronic RfD is unnecessarily conservative.

In their analysis of the issue, the SAB indicates that, for most chemicals, the approach of combining the higher 6-year exposure for children with chronic toxicity criteria is overly protective (U.S. EPA, 1993e). However, they noted that there are instances when the chronic RfD may be based on endpoints of toxicity that are specific to children (e.g., fluoride and nitrates) or when the dose-response curve is steep (i.e., the dosage difference between the no-observed-adverse-effects level [NOAEL] and an adverse effects level is small). Thus, for the purposes of screening, OERR opted to base the generic SSLs for noncarcinogenic contaminants on the more conservative “childhood only” exposure (Equation 1). The issue of whether to maintain this more conservative approach throughout the baseline risk assessment and establishing remediation goals will depend on how the toxicology of the chemical relates to the issues raised by the SAB.

Screening Level Equation for Ingestion of Noncarcinogenic Contaminants in Residential Soil

(Source: RAGS HHEM, Part B; U.S. EPA, 1991b)

$$\text{Screening Level (mg/kg)} = \frac{\text{THQ} \times \text{BW} \times \text{AT} \times 365\ \text{d/yr}}{1/\text{RfD}_o \times 10^{-6}\ \text{kg/mg} \times \text{EF} \times \text{ED} \times \text{IR}} \tag{1}$$

Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
BW/body weight (kg)	15
AT/averaging time (yr)	6[a]
RfD_o /oral reference dose (mg/kg-d)	chemical-specific
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	6
IR/soil ingestion rate (mg/d)	200

[a] For noncarcinogens, averaging time is equal to exposure duration. Unlike RAGS HHEM, Part B, SSLs are calculated only for 6-year childhood exposure.

For carcinogens, both the magnitude and duration of exposure are important. Duration is critical because the toxicity criteria are based on "lifetime average daily dose." Therefore, the total dose received, whether it be over 5 years or 50 years, is averaged over a lifetime of 70 years. To be protective of exposures to carcinogens in the residential setting, RAGS HHEM, Part B (U.S. EPA, 1991b) and EPA focus on exposures to individuals who may live in the same residence for a "high-end" period of time (e.g., 30 years). As mentioned above, exposure to soil is higher during childhood and decreases with age. Thus, Equation 2 uses the RAGS HHEM, Part B time-weighted average soil ingestion rate for children and adults; the derivation of this factor is shown in Equation 3.

Screening Level Equation for Ingestion of Carcinogenic Contaminants in Residential Soil

(Source: RAGS HHEM, Part B; U.S. EPA, 1991b)

$$\text{Screening Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365\ \text{d/yr}}{\text{SF}_o \times 10^{-6}\ \text{kg/mg} \times \text{EF} \times \text{IF}_{\text{soil/adj}}} \tag{2}$$

Parameter/Definition (units)	Default
TR/target cancer risk (unitless)	10^{-6}
AT/averaging time (yr)	70
SF_o /oral slope factor $(mg/kg\text{-}d)^{-1}$	chemical-specific
EF/exposure frequency (d/yr)	350
$IF_{soil/adj}$ /age-adjusted soil ingestion factor (mg-yr/kg-d)	114

Equation for Age-Adjusted Soil Ingestion Factor, $IF_{soil/adj}$

$$\frac{IF_{soil/adj}}{(mg\text{-}yr/kg\text{-}d)} = \frac{IR_{soil/age1\text{-}6} \times ED_{age1\text{-}6}}{BW_{age1\text{-}6}} + \frac{IR_{soil/age7\text{-}31} \times ED_{age7\text{-}31}}{BW_{age7\text{-}31}} \qquad (3)$$

Parameter/Definition (units)	Default
$IF_{soil/adj}$ /age-adjusted soil ingestion factor (mg-yr/kg-d)	114
$IR_{soil/age1\text{-}6}$ /ingestion rate of soil age 1-6 (mg/d)	200
$ED_{age1\text{-}6}$ /exposure duration during ages 1-6 (yr)	6
$IR_{soil/age7\text{-}31}$ /ingestion rate of soil age 7-31 (mg/d)	100
$ED_{age7\text{-}31}$ /exposure duration during ages 7-31 (yr)	24
$BW_{age1\text{-}6}$ /average body weight from ages 1-6 (kg)	15
$BW_{age7\text{-}31}$ /average body weight from ages 7-31 (kg)	70

Source: RAGS HHEM, Part B (U.S. EPA, 1991b).

Because of the impracticability of developing site-specific input parameters (e.g., soil ingestion rates, chemical-specific bioavailability) for direct soil ingestion, SSLs are calculated using the defaults listed in Equations 1, 2, and 3. Appendix A lists these generic SSLs for direct ingestion of soil.

2.3 Dermal Absorption

Incorporation of dermal exposures into the Soil Screening Guidance is limited by the amount of data available to quantify dermal absorption from soil for specific chemicals. EPA's ORD evaluated the available data on absorption of chemicals from soil in the document *Dermal Exposure Assessment: Principles and Applications* (U.S. EPA, 1992b). This document also presents calculations comparing the potential dose of a chemical in soil from oral routes with that from dermal routes of exposure.

These calculations suggest that, assuming 100 percent absorption of a chemical via ingestion, absorption via the dermal route must be greater than 10 percent to equal or exceed the ingestion exposure. Of the 110 compounds evaluated, available data are adequate to show greater than 10 percent dermal absorption only for pentachlorophenol (Wester et al., 1993). Therefore, the ingestion SSL for pentachlorophenol is adjusted to account for this additional exposure (i.e., the ingestion SSL has been divided in half to account for increased exposure via the dermal route). Limited data suggest that dermal absorption of other semivolatile organic chemicals (e.g., benzo(*a*)pyrene) from soil may exceed 10 percent (Wester et al., 1990) but EPA believes that further investigation is needed. As adequate dermal absorption data are developed for such chemicals the ingestion SSLs may need to be adjusted. EPA will provide updates on this issue as appropriate.

2.4 Inhalation of Volatiles and Fugitive Dusts

EPA toxicity data indicate that risks from exposure to some chemicals via inhalation far outweigh the risks via ingestion; therefore, the SSLs have been designed to address this pathway as well. The models and assumptions used to calculate SSLs for inhalation of volatiles are updates of risk assessment methods presented in RAGS HHEM, Part B (U.S. EPA, 1991b). RAGS HHEM, Part B evaluated the contribution to risk from the inhalation and ingestion pathways simultaneously. Because toxicity criteria for oral exposures are presented as administered doses (in mg/kg-d) and criteria for inhalation exposures are presented as concentrations in air (in $\mu g/m^3$), conversion of air concentrations was required to estimate an administered dose comparable to the oral route. However, EPA's ORD now believes that, due to portal-of-entry effects and differences in absorption in the gut versus the lungs, the conversion from concentration in air to internal dose is not always appropriate and suggests evaluating these exposure routes separately.

The models and assumptions used to calculate SSLs for the inhalation pathway are presented in Equations 4 through 12, along with the default parameter values used to calculate the generic SSLs presented in Appendix A. Particular attention is given to the volatilization factor (VF), saturation limit (C_{sat}), and the dispersion portion of the VF and particulate emission factor (PEF) equations, all of which have been revised since originally presented in RAGS HHEM, Part B. The available chemical-specific human health benchmarks used in these equations are presented in Section 2.1. Part 5 presents the chemical properties required by these equations, along with the rationale for their selection and development.

2.4.1 Screening Level Equations for Direct Inhalation. Equations 4 and 5 are used to calculate SSLs for the inhalation of carcinogenic and noncarcinogenic contaminants, respectively. Each equation addresses volatile compounds and fugitive dusts separately for developing screening levels based on inhalation risk for subsurface soils and surface soils.

Separate VF-based and PEF-based equations were developed because the SSL sampling strategy addresses surface and subsurface soils separately. Inhalation risk from fugitive dusts results from particle entrainment from the soil surface; thus contaminant concentrations in the surface soil horizon (e.g., the top 2 centimeters) are of primary concern for this pathway. The entire column of contaminated soil can contribute to volatile emissions at a site. However, the top 2 centimeters are likely to be depleted of volatile contaminants at most sites. Thus, contaminant concentrations in subsurface soils, which are measured using core samples, are of primary concern for quantifying the risk from volatile emissions.

Screening Level Equation for Inhalation of Carcinogenic Contaminants in Residential Soil

$$\text{Volatile Screening Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365\ \text{d/yr}}{\text{URF} \times 1{,}000\ \mu\text{g/mg} \times \text{EF} \times \text{ED} \times \left[\frac{1}{\text{VF}}\right]} \qquad \textbf{(4)}$$

$$\text{Particulate Screening Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365\ \text{d/yr}}{\text{URF} \times 1{,}000\ \mu\text{g/mg} \times \text{EF} \times \text{ED} \times \left[\frac{1}{\text{PEF}}\right]}$$

Parameter/Definition (units)	Default
TR/target cancer risk (unitless)	10^{-6}
AT/averaging time (yr)	70
URF/inhalation unit risk factor (μg/m^3)$^{-1}$	chemical-specific
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	30
VF/soil-to-air volatilization factor (m^3/kg)	chemical-specific
PEF/particulate emission factor (m^3/kg)	1.32×10^9

Source: RAGS HHEM, Part B (U.S. EPA, 1991b).

Screening Level Equation for Inhalation of Noncarcinogenic Contaminants in Residential Soil

$$\text{Volatile Screening Level (mg/kg)} = \frac{\text{THQ} \times \text{AT} \times 365\ \text{d/yr}}{\text{EF} \times \text{ED} \times \left(\frac{1}{\text{RfC}} \times \frac{1}{\text{VF}}\right)} \qquad \textbf{(5)}$$

$$\text{Particulate Screening Level (mg/kg)} = \frac{\text{THQ} \times \text{AT} \times 365\ \text{d/yr}}{\text{EF} \times \text{ED} \times \left(\frac{1}{\text{RfC}} \times \frac{1}{\text{PEF}}\right)}$$

Parameter/Definition (units)	Default
THQ/target hazard quotient (unitless)	1
AT/averaging time (yr)	30
EF/exposure frequency (d/yr)	350
ED/exposure duration (yr)	30
RfC/inhalation reference concentration (mg/m^3)	chemical-specific
VF/soil-to-air volatilization factor (m^3/kg)	chemical-specific
PEF/particulate emission factor (m^3/kg) (Equation 10)	1.32 x 10^9

Source: RAGS HHEM, Part B (U.S. EPA, 1991b).

To calculate inhalation SSLs, the volatilization factor and particulate emission factor must be calculated. The derivations of VF and PEF have been updated since RAGS HHEM, Part B was published and are discussed fully in Sections 2.4.2 and 2.4.5, respectively. The VF and PEF equations can be broken into two separate models: models to estimate the emissions of volatiles and dusts, and a dispersion model (reduced to the term Q/C) that simulates the dispersion of contaminants in the atmosphere.

2.4.2 Volatilization Factor. The soil-to-air VF is used to define the relationship between the concentration of the contaminant in soil and the flux of the volatilized contaminant to air. VF is calculated from Equation 6 using chemical-specific properties (see Part 5) and either site-measured or default values for soil moisture, dry bulk density, and fraction of organic carbon in soil. The User's Guide (U.S. EPA, 1996) describes how to develop site measured values for these parameters.

Derivation of Volatilization Factor

(6)

$$\mathrm{VF}\,(\mathrm{m}^3/\mathrm{kg}) = Q/C \times \frac{(3.14 \times D_A \times T)^{1/2}}{(2 \times \rho_b \times D_A)} \times 10^{-4}(\mathrm{m}^2/\mathrm{cm}^2)$$

where

$$D_A = \frac{\left[(\theta_a^{10/3} D_i\, H' + \theta_w^{10/3}\, D_w)/n^2\right]}{\rho_b\, K_d + \theta_w + \theta_a\, H'}$$

Parameter/Definition (units)	Default	Source
VF/volatilization factor (m^3/kg)	–	–
D_A /apparent diffusivity (cm^2/s)	–	–
Q/C/inverse of the mean conc. at center of square source (g/m^2-s per kg/m^3)	68.81	Table 3 (for 0.5-acre source in Los Angeles, CA)
T/exposure interval (s)	9.5×10^8	U.S. EPA (1991b)
ρ_b/dry soil bulk density (g/cm^3)	1.5	U.S. EPA (1991b)
θ_a /air-filled soil porosity (L_{air}/L_{soil})	0.28	n - θ_w
n/total soil porosity (L_{pore}/L_{soil})	0.43	1 - (ρ_b/ρ_s)
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.15	EQ, 1994
ρ_s /soil particle density (g/cm^3)	2.65	U.S. EPA (1991b)
D_i /diffusivity in air (cm^2/s)	chemical-specific	see Part 5
H′/dimensionless Henry's law constant	chemical-specific	see Part 5
D_w /diffusivity in water (cm^2/s)	chemical-specific	see Part 5
K_d /soil-water partition coefficient (cm^3/g) = K_{oc} f_{oc}	chemical-specific	see Part 5
K_{oc} /soil organic carbon-water partition coefficient (cm^3/g)	chemical-specific	see Part 5
f_{oc}/organic carbon content of soil (g/g)	0.006 (0.6%)	Carsel et al. (1988)

The VF equation presented in Equation 6 is based on the volatilization model developed by Jury et al. (1984) for infinite sources and is theoretically consistent with the Jury et al. (1990) finite source volatilization model (see Section 3.1). This equation represents a change in the fundamental volatilization model used to derive the VF equation used in RAGS HHEM, Part B and in the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h).

The VF equation presented in RAGS HHEM, Part B is based on the volatilization model developed by Hwang and Falco (1986) for dry soils. During the reevaluation of RAGS HHEM, Part B, EPA sponsored a study (see the December 1994 draft Technical Background Document, U.S. EPA, 1994i) to validate the VF equation by comparing the modeled results with data from (1) a bench-scale pesticide study (Farmer and Letey, 1974) and (2) a pilot-scale study measuring the rate of loss of benzene, toluene, xylenes, and ethylbenzene from soils using an isolation flux chamber (Radian, 1989). The results of the study verified the need to modify the VF equation in Part B to take into account the decrease in the rate of flux due to the effect of soil moisture content on effective diffusivity (D_{ei}).

In the December 1994 version of this background document (U.S. EPA, 1994i), the Hwang and Falco model was modified to account for the influence of soil moisture on the effective diffusivity using the Millington and Quirk (1961) equation. However, inconsistencies were discovered in the modified Hwang and Falco equations. Additionally, even a correctly modified Hwang and Falco model does not consider the influence of the liquid phase on the local equilibrium partitioning. Consequently, EPA evaluated the Jury model for its ability to predict emissions measured in pilot-scale volatilization studies (Appendix C; EQ, 1995). The infinite source Jury model emission rate predictions were consistently within a factor of 2 of the emission rates measured in the pilot-scale volatilization studies. Because the Jury model predicts well the available measured soil contaminant volatilization rates, eliminates the inconsistencies of the modified Hwang and Falco model, and considers the influence of the liquid phase on the local equilibrium partitioning, it was selected to replace the modified Hwang and Falco model for the derivation of the VF equation.

Defaults. Other than initial soil concentration, air-filled soil porosity is the most significant soil parameter affecting the final steady-state flux of volatile contaminants from soil (U.S. EPA, 1980). In other words, the higher the air-filled soil porosity, the greater the emission flux of volatile constituents. Air-filled soil porosity is calculated as:

$$\theta_a = n - \theta_w \tag{7}$$

where

θ_a = air-filled soil porosity (L_{air}/L_{soil})
n = total soil porosity (L_{pore}/L_{soil})
θ_w = water-filled soil porosity (L_{water}/L_{soil})

and

$$n = 1 - (\rho_b/\rho_s) \tag{8}$$

where

ρ_b = dry soil bulk density (g/cm^3)
ρ_s = soil particle density (g/cm^3).

Of these parameters, water-filled soil porosity (θ_w) has the most significant effect on air-filled soil porosity and hence volatile contaminant emissions. Sensitivity analyses have shown that soil bulk density (ρ_b) has too limited a range for surface soils (generally between 1.3 and 1.7 g/cm^3) to affect results with nearly the significance of soil moisture conditions. Therefore, a default bulk density of 1.50 g/cm^3, the mode of the range given for U.S. soils in the *Superfund Exposure Assessment Manual* (U.S. EPA, 1988), was chosen to calculate generic SSLs. This value is also consistent with the mean porosity (0.43) for loam soil presented in Carsel and Parrish (1988).

The default value of θ_w (0.15) corresponds to an average annual soil water content of 10 weight percent. This value was chosen as a conservative compromise between that required to achieve a monomolecular layer of water on soil particles (approximately 2 to 5 weight percent) and that required to reduce the air-filled porosity to zero (approximately 29 weight percent). In this manner, nonpolar or weakly polar contaminants are desorbed readily from the soil organic carbon as water competes for sorption sites. At the same time, a soil moisture content of 10 percent yields a relatively conservative air-filled porosity (0.28 or 28 percent by volume). A water-filled soil porosity (θ_w) of 0.15 lies about halfway between the mean wilting point (0.09) and mean field capacity (0.20) reported for Class B soils by Carsel et al. (1988). Class B soils are soils with moderate hydrologic characteristics whose average characteristics are well represented by a loam soil type.

The default value of ρ_s (2.65 g/cm^3) was taken from U.S. EPA (1988) as the particle density for most soil mineral material. The default value for f_{oc} (0.006 or 0.6 percent) is the mean value for the top 0.3 m of Class B soils from Carsel et al. (1988).

2.4.3 Dispersion Model. The box model in RAGS HHEM, Part B has been replaced with a Q/C term derived from a modeling exercise using meteorologic data from 29 locations across the United States.

The dispersion model used in the Part B guidance is based on the assumption that emissions into a hypothetical box will be distributed uniformly throughout the box. To arrive at the volume within the box, it is necessary to assign values to the length, width, and height of the box. The length (LS) was the length of a side of a contaminated site with a default value of 45 m; the width was based on the windspeed in the mixing zone (V) with a default value of 2.25 m (based on a windspeed of 2.25 m/s); and the height was the diffusion height (DH) with a default value of 2 m.

However, the assumptions and mathematical treatment of dispersion used in the box model may not be applicable to a broad range of site types and meteorology and do not utilize state-of-the-art techniques developed for regulatory dispersion modeling. EPA was very concerned about the defensibility of the box model and sought a more defensible dispersion model that could be used as a replacement to the Part B guidance and had the following characteristics:

- Dispersion modeling from a ground-level area source
- Onsite receptor
- A long-term/annual average exposure point concentration
- Algorithms for calculating the exposure point concentration for area sources of different sizes and shapes.

To identify such a model, EPA held discussions with the EPA Office of Air Quality Planning and Standards (OAQPS) concerning recent efforts to develop a new algorithm for estimating ambient air concentrations from low or ground-level, nonbuoyant sources of emissions. The new algorithm is incorporated into the Industrial Source Complex Model (ISC2) platform in both a short-term mode (AREA-ST) and a long-term mode (AREA-LT). Both models employ a double numerical integration over the source in the upwind and crosswind directions. Wind tunnel tests have shown that the new algorithm performs well with onsite and near-field receptors. In addition, subdivision of the source is not required for these receptors.

Because the new algorithm provides better concentration estimates for onsite and for near-field receptors, a revised dispersion analysis was performed for both volatile and particulate matter contaminants (Appendix D; EQ, 1994). The AREA-ST model was run for 0.5-acre and 30-acre square sources with a full year of meteorologic data for 29 U.S locations selected to be representative of the national range of meteorologic conditions (EQ, 1993). Additional modeling runs were conducted to address a range of square area sources from 0.5 to 30 acres in size (Table 3). The Q/C values in Table 3 for 0.5- and 30-acre sources differ slightly from the values in Appendix D due to differences in rounding conventions used in the final model runs.

To calculate site-specific SSLs, select a Q/C value from Table 3 that best represents a site's size and meteorologic condition.

To develop a reasonably conservative default Q/C for calculating generic SSLs, a default site (Los Angeles, CA) was chosen that best approximated the 90th percentile of the 29 normalized concentrations (kg/m^3 per g/m^2-s). The inverse of this concentration results in a default VF Q/C value of 68.81 g/m^2-s per kg/m^3 for a 0.5-acre site.

Table 3. Q/C Values by Source Area, City, and Climatic Zone

	Q/C (g/m^2-s per kg/m^3)					
	0.5 Acre	**1 Acre**	**2 Acre**	**5 Acre**	**10 Acre**	**30 Acre**
Zone I						
Seattle	82.72	72.62	64.38	55.66	50.09	42.86
Salem	73.44	64.42	57.09	49.33	44.37	37.94
Zone II						
Fresno	62.00	54.37	48.16	41.57	37.36	31.90
Los Angeles	68.81	60.24	53.30	45.93	41.24	35.15
San Francisco	89.51	78.51	69.55	60.03	53.95	46.03
Zone III						
Las Vegas	95.55	83.87	74.38	64.32	57.90	49.56
Phoenix	64.04	56.07	49.59	42.72	38.35	32.68
Albuquerque	84.18	73.82	65.40	56.47	50.77	43.37
Zone IV						
Boise	69.41	60.88	53.94	46.57	41.87	35.75
Winnemucca	69.23	60.67	53.72	46.35	41.65	35.55
Salt Lake City	78.09	68.47	60.66	52.37	47.08	40.20
Casper	100.13	87.87	77.91	67.34	60.59	51.80
Denver	75.59	66.27	58.68	50.64	45.52	38.87
Zone V						
Bismark	83.39	73.07	64.71	55.82	50.16	42.79
Minneapolis	90.80	79.68	70.64	61.03	54.90	46.92
Lincoln	81.64	71.47	63.22	54.47	48.89	41.65
Zone VI						
Little Rock	73.63	64.51	57.10	49.23	44.19	37.64
Houston	79.25	69.47	61.53	53.11	47.74	40.76
Atlanta	77.08	67.56	59.83	51.62	46.37	39.54
Charleston	74.89	65.65	58.13	50.17	45.08	38.48
Raleigh-Durham	77.26	67.75	60.01	51.78	46.51	39.64
Zone VII						
Chicago	97.78	85.81	76.08	65.75	59.16	50.60
Cleveland	83.22	73.06	64.78	55.99	50.38	43.08
Huntington	53.89	47.24	41.83	36.10	32.43	27.67
Harrisburg	81.90	71.87	63.72	55.07	49.56	42.40
Zone VIII						
Portland	74.23	65.01	57.52	49.57	44.49	37.88
Hartford	71.35	62.55	55.40	47.83	43.00	36.73
Philadelphia	90.24	79.14	70.14	60.59	54.50	46.59
Zone IX						
Miami	85.61	74.97	66.33	57.17	51.33	43.74

2.4.4 Soil Saturation Limit.

The soil saturation concentration (C_{sat}) corresponds to the contaminant concentration in soil at which the absorptive limits of the soil particles, the solubility limits of the soil pore water, and saturation of soil pore air have been reached. Above this concentration, the soil contaminant may be present in free phase, i.e., nonaqueous phase liquids (NAPLs) for contaminants that are liquid at ambient soil temperatures and pure solid phases for compounds that are solid at ambient soil temperatures.

Derivation of the Soil Saturation Limit

$$C_{sat} = \frac{S}{\rho_b}\left(K_d\,\rho_b + \theta_w + H'\,\theta_a\right) \tag{9}$$

Parameter/Definition (units)	Default	Source
C_{sat}/soil saturation concentration (mg/kg)	–	
S/solubility in water (mg/L-water)	chemical-specific	see Part 5
ρ_b/dry soil bulk density (kg/L)	1.5	U.S. EPA, 1991b
K_d/soil-water partition coefficient (L/kg)	$K_{oc} \times f_{oc}$ (organics)	
K_{oc}/soil organic carbon/water partition coefficient (L/kg)	chemical-specific	see Part 5
f_{oc}/fraction organic carbon of soil (g/g)	0.006 (0.6%)	Carsel et al., 1988
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.15	EQ, 1994
H′/dimensionless Henry's law constant	H x 41, where 41 is a conversion factor	U.S. EPA, 1991b
H/Henry's law constant (atm-m^3/mol)	chemical-specific	see Part 5
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.28	$n - \theta_w$
n/total soil porosity (L_{pore}/L_{soil})	0.43	$1 - \rho_b/\rho_s$
ρ_s/soil particle density (kg/L)	2.65	U.S. EPA, 1991b

Equation 9 is used to calculate C_{sat} for each site contaminant. As an update to RAGS HHEM, Part B, this equation takes into account the amount of contaminant that is in the vapor phase in the pore spaces of the soil in addition to the amount dissolved in the soil's pore water and sorbed to soil particles.

Chemical-specific C_{sat} concentrations must be compared with each volatile inhalation SSL because a basic principle of the SSL volatilization model (Henry's law) is not applicable when free-phase contaminants are present (i.e., the model cannot predict an accurate VF or SSL above C_{sat}). Thus, the VF-based inhalation SSLs are applicable only if the soil concentration is at or below C_{sat}. When calculating volatile inhalation SSLs, C_{sat} values also should be calculated using the same site-specific soil characteristics used to calculate SSLs (i.e., bulk density, average water content, and organic carbon content).

At C_{sat} the emission flux from soil to air for a chemical reaches a plateau. Volatile emissions will not increase above this level no matter how much more chemical is added to the soil. Table 3-A shows that for compounds with generic volatile inhalation SSLs greater than C_{sat}, the risks at C_{sat} are significantly below the screening risk of 1 x 10^{-6} and an HQ of 1. Since C_{sat} corresponds to maximum volatile emissions, the inhalation route is not likely to be of concern for those chemicals with SSLs exceeding C_{sat} concentrations.

Table 3-A. Risk Levels Calculated at C_{sat} for Contaminants that have SSL_{inh} Values Greater than C_{sat}

Chemical name	URF $(\mu g/m^3)^{-1}$	RfC (mg/m^3)	VF (m^3/kg)	C_{sat} (mg/kg)	Carcinogenic Risk	Non-Carcinogenic Risk
DDT	9.7E-05	---	3.0E+07	4.0E+02	5.2E-07	---
1,2-Dichlorobenzene	---	2.0E-01	1.5E+04	6.0E+02	---	0.2
1,4-Dichlorobenzene	---	8.0E-01	1.3E+04	2.8E+02	---	0.03
Ethylbenzene	---	1.0E+00	5.4E+03	4.0E+02	---	0.07
β-HCH (β-BHC)	5.3E-04	---	1.3E+06	2.0E+00	3.4E-07	---
Styrene	---	1.0E+00	1.3E+04	1.5E+03	---	0.1
Toluene	---	4.0E-01	4.0E+03	6.5E+02	---	0.4
1,2,4-Trichlorobenzene	---	2.0E-01	4.3E+04	3.2E+03	---	0.4
1,1,1-Trichloroethane	---	1.0E+00	2.2E-03	1.2E+03	---	0.5

Table 4 provides the physical state (i.e. liquid or solid) for various compounds at ambient soil temperature. When the inhalation SSL exceeds C_{sat} for liquid compounds, the SSL is set at C_{sat}. This is because, for compounds that are liquid at ambient soil temperature, concentrations above C_{sat} indicate a potential for free liquid phase contamination to be present, and the possible presence of NAPLs. EPA believes that further investigation is warranted when free nonaqueous phase liquids may be present in soils at a site.

Table 4. Physical State of Organic SSL Chemicals

Compounds liquid at soil temperatures			Compounds solid at soil temperatures		
CAS No.	Chemical	Melting Point (˚C)	CAS No.	Chemical	Melting Point (˚C)
67-64-1	Acetone	-94.8	83-32-9	Acenaphthene	93.4
71-43-2	Benzene	5.5	309-00-2	Aldrin	104
117-81-7	Bis(2-ethylhexyl)phthalate	-55	120-12-7	Anthracene	215
111-44-4	Bis(2-chloroethyl)ether	-51.9	56-55-3	Benz(*a*)anthracene	84
75-27-4	Bromodichloromethane	-57	50-32-8	Benzo(*a*)pyrene	176.5
75-25-2	Bromoform	8	205-99-2	Benzo(*b*)fluoranthene	168
71-36-3	Butanol	-89.8	207-08-9	Benzo(*k*)fluoranthene	217
85-68-7	Butyl benzyl phthalate	-35	65-85-0	Benzoic acid	122.4
75-15-0	Carbon disulfide	-115	86-74-8	Carbazole	246.2
56-23-5	Carbon tetrachloride	-23	57-74-9	Chlordane	106
108-90-7	Chlorobenzene	-45.2	106-47-8	*p*-Chloroaniline	72.5
124-48-1	Chlorodibromomethane	-20	218-01-9	Chrysene	258.2
67-66-3	Chloroform	-63.6	72-54-8	DDD	109.5

Table 4. (continued)

Compounds liquid at soil temperatures			Compounds solid at soil temperatures		
CAS No.	Chemical	Melting Point (˚C)	CAS No.	Chemical	Melting Point (˚C)
95-57-8	2-Chlorophenol	9.8	72-55-9	DDE	89
84-74-2	Di-*n*-butyl phthalate	-35	50-29-3	DDT	108.5
95-50-1	1,2-Dichlorobenzene	-16.7	53-70-3	Dibenzo(*a,h*)anthracene	269.5
75-34-3	1,1-Dichloroethane	-96.9	106-46-7	1,4-Dichlorobenzene	52.7
107-06-2	1,2-Dichloroethane	-35.5	91-94-1	3,3-Dichlorobenzidine	132.5
75-35-4	1,1-Dichloroethylene	-122.5	120-83-2	2,4-Dichlorophenol	45
156-59-2	*cis*-1,2-Dichloroethylene	-80	60-57-1	Dieldrin	175.5
156-60-5	*trans*-1,2-Dichloroethylene	-49.8	105-67-9	2,4-Dimethylphenol	24.5
78-87-5	1,2-Dichloropropane	-70	51-28-5	2,4-Dinitrophenol	115-116
542-75-6	1,3-Dichloropropene	NA	121-14-2	2,4-Dinitrotoluene	71
84-66-2	Diethylphthalate	-40.5	606-20-2	2,6-Dinitrotoluene	66
117-84-0	Di-*n*-octyl phthalate	-30	72-20-8	Endrin	200
100-41-4	Ethylbenzene	-94.9	206-44-0	Fluoranthene	107.8
87-68-3	Hexachloro-1,3-butadiene	-21	86-73-7	Fluorene	114.8
77-47-4	Hexachlorocyclopentadiene	-9	76-44-8	Heptachlor	95.5
78-59-1	Isophorone	-8.1	1024-57-3	Heptachlor epoxide	160
74-83-9	Methyl bromide	-93.7	118-74-1	Hexachlorobenzene	231.8
75-09-2	Methylene chloride	-95.1	319-84-6	α-HCH (α-BHC)	160
98-95-3	Nitrobenzene	5.7	319-85-7	ß-HCH (ß-BHC)	315
100-42-5	Styrene	-31	58-89-9	γ-HCH (Lindane)	112.5
79-34-5	1,1,2,2-Tetrachloroethane	-43.8	67-72-1	Hexachloroethane	187
127-18-4	Tetrachloroethylene	-22.3	193-39-5	Indeno(1,2,3-*cd*)pyrene	161.5
108-88-3	Toluene	-94.9	72-43-5	Methoxychlor	87
120-82-1	1,2,4-Trichlorobenzene	17	95-48-7	2-Methylphenol	29.8
71-55-6	1,1,1-Trichloroethane	-30.4	621-64-7	*N*-Nitrosodi-*n*-propylamine	NA
79-00-5	1,1,2-Trichloroethane	-36.6	86-30-6	*N*-Nitrosodiphenylamine	66.5
79-01-6	Trichloroethylene	-84.7	91-20-3	Naphthalene	80.2
108-05-4	Vinyl acetate	-93.2	87-86-5	Pentachlorophenol	174
75-01-4	Vinyl chloride	-153.7	108-95-2	Phenol	40.9
108-38-3	*m*-Xylene	-47.8	129-00-0	Pyrene	151.2
95-47-6	*o*-Xylene	-25.2	8001-35-2	Toxaphene	65-90
106-42-3	*p*-Xylene	13.2	95-95-4	2,4,5-Trichlorophenol	69
			88-06-2	2,4,6-Trichlorophenol	69
			115-29-7	Endosullfan	106

NA = Not available.

When free phase liquid contaminants are suspected, *Estimating the Potential for Occurrence of DNAPL at Superfund Sites* (U.S. EPA, 1992c) provides information on determining the likelihood of dense nonaqueous phase liquid (DNAPL) occurrence in the subsurface. Free-phase contaminants may also be present at concentrations lower than C_{sat} if multiple component mixtures are present. The DNAPL guidance (U.S. EPA, 1992c) also addresses the likelihood of free-phase contaminants when multiple contaminants are present at a site.

For compounds that are solid at ambient soil temperatures (e.g., DDT), Table 3-A indicates that the inhalation risks are well below the screening targets (i.e., these chemicals do not appear to be of concern for the inhalation pathway). Thus, when inhalation SSLs are above C_{sat} for solid compounds, soil screening decisions should be based on the appropriate SSLs for other pathways of concern at the site (e.g., migration to ground water, ingestion).

2.4.5 Particulate Emission Factor. The particulate emission factor relates the concentration of contaminant in soil with the concentration of dust particles in the air. This guidance addresses dust generated from open sources, which is termed "fugitive" because it is not discharged into the atmosphere in a confined flow stream. Other sources of fugitive dusts that may lead to higher emissions due to mechanical disturbances include unpaved roads, tilled agricultural soils, and heavy construction operations.

Both the emissions portion and the dispersion portion of the PEF equation have been updated since RAGS HHEM, Part B.

As in Part B, the emissions part of the PEF equation is based on the "unlimited reservoir" model from Cowherd et al. (1985) developed to estimate particulate emissions due to wind erosion. The unlimited reservoir model is most sensitive to the threshold friction velocity, which is a function of the mode of the size distribution of surface soil aggregates. This parameter has the greatest effect on the emissions and resulting concentration. For this reason, a conservative mode soil aggregate size of 500 µm was selected as the default value for calculating generic SSLs.

The mode soil aggregate size determines how much wind is needed before dust is generated at a site. A mode soil aggregate size of 500 µm yields an **uncorrected** threshold friction velocity of 0.5 m/s. This means that the windspeed must be at least 0.5 m/s before any fugitive dusts are generated. However, the threshold friction velocity **should be corrected** to account for the presence of nonerodible elements. In Cowherd et al. (1985), nonerodible elements are described as

> . . . clumps of grass or stones (larger than about 1 cm in diameter) on the surface (that will) consume part of the shear stress of the wind which otherwise would be transferred to erodible soil.

Cowherd et al. describe a study by Marshall (1971) that used wind tunnel studies to quantify the increase in the threshold friction velocity for different kinds of nonerodible elements. His results are presented in Cowherd et al. as a graph showing the rate of corrected to uncorrected threshold friction velocity vs. L_c, where L_c is a measure of nonerodible elements vs. bare, loose soil. Thus, the ratio of corrected to uncorrected threshold friction velocity is directly related to the amount of nonerodible elements in surface soils.

Using a ratio of corrected to uncorrected threshold friction velocity of 1, or no correction, is roughly equivalent to modeling "coal dust on a concrete pad," whereas using a correction factor of 2 corresponds to a windspeed of 19 m/s at a height of 10 m. This means that about a 43-mph wind would be required to produce any particulate emissions. Given that the 29 meteorologic data sets used in this modeling effort showed few windspeeds at, or greater than, 19 m/s, EPA felt that it was necessary to choose a default correction ratio between 1 and 2. A value of 1.25 was selected as a reasonable number that would be at the more conservative end of the range. This equates to a corrected threshold friction velocity of 0.625 m/s and an equivalent windspeed of 11.3 m/s at a height of 7 meters.

As with the VF model, Q/C values are needed to calculate the PEF (Equation 10); use the QC value in Table 3 that best represents a site's size and meteorologic conditions (i.e., the same value used to calculate the VF; see Section 2.4.2). Cowherd et al. (1985) describe how to obtain site-specific estimates of V, U_m, U_t, and F(x).

Unlike volatile contaminants, meteorologic conditions (i.e., the intensity and frequency of wind) affect both the dispersion and emissions of particulate matter. For this reason, a separate default Q/C value was derived for particulate matter [nominally 10 µm and less (PM_{10})] emissions for the generic SSLs. The PEF equation was used to calculate annual average concentrations for each of 29 sites across the country. To develop a reasonably conservative default Q/C for calculating generic SSLs, a default site (Minneapolis, MN) was selected that best approximated the 90th percentile concentration.

The results produced a revised default PEF Q/C value of 90.80 g/m^2-s per kg/m^3 for a 0.5-acre site (see Appendix D; EQ, 1994). The generic PEF derived using the default values in Equation 10 is 1.32×10^9 m^3/kg, which corresponds to a receptor point concentration of approximately 0.76 $\mu g/m^3$. This represents an annual average emission rate based on wind erosion that should be compared with chronic health criteria; it is **not** appropriate for evaluating the potential for more acute exposures.

Derivation of the Particulate Emission Factor

$$\mathrm{PEF}\ (\mathrm{m}^3/\mathrm{kg}) = Q/C \times \frac{3{,}600\ \mathrm{s/h}}{0.036 \times (1-V) \times (U_m/U_t)^3 \times F(x)} \qquad \mathbf{(10)}$$

Parameter/Definition (units)	Default	Source
PEF/particulate emission factor (m^3/kg)	1.32×10^9	--
Q/C/inverse of mean conc. at center of square source (g/m^2-s per kg/m^3)	90.80	Table 3 (for 0.5-acre source in Minneapolis, MN)
V/fraction of vegetative cover (unitless)	0.5 (50%)	U.S. EPA, 1991b
U_m/mean annual windspeed (m/s)	4.69	EQ, 1994
U_t/equivalent threshold value of windspeed at 7 m (m/s)	11.32	U.S. EPA, 1991b
F(x)/function dependent on U_m/U_t derived using Cowherd et al. (1985) (unitless)	0.194	U.S. EPA, 1991b

2.5 Migration to Ground Water

The methodology for calculating SSLs for the migration to ground water pathway was developed to identify chemical concentrations in soil that have the potential to contaminate ground water.

Migration of contaminants from soil to ground water can be envisioned as a two-stage process: (1) release of contaminant in soil leachate and (2) transport of the contaminant through the underlying soil and aquifer to a receptor well. The SSL methodology considers both of these fate and transport mechanisms.

The methodology incorporates a standard linear equilibrium soil/water partition equation to estimate contaminant release in soil leachate (see Sections 2.5.1 through 2.5.4) and a simple water-balance equation that calculates a dilution factor to account for dilution of soil leachate in an aquifer (see Section 2.5.5). The dilution factor represents the reduction in soil leachate contaminant concentrations by mixing in the aquifer, expressed as the ratio of leachate concentration to the concentration in ground water at the receptor point (i.e., drinking water well). Because the infinite source assumption can result in mass-balance violations for soluble contaminants and small sources, mass-limit models are provided that limit the amount of contaminant migrating from soil to ground water to the total amount of contaminant present in the source (see Section 2.6).

SSLs are backcalculated from acceptable ground water concentrations (i.e., nonzero MCLGs, MCLs, or HBLs; see Section 2.1). First, the acceptable ground water concentration is multiplied by a dilution factor to obtain a target leachate concentration. For example, if the dilution factor is 10 and the acceptable ground water concentration is 0.05 mg/L, the target soil leachate concentration would be 0.5 mg/L. The partition equation is then used to calculate the total soil concentration (i.e., SSL) corresponding to this soil leachate concentration.

The methodology for calculating SSLs for the migration to ground water pathway was developed under the following constraints:

- Because of the large nationwide variability in ground water vulnerability, the methodology should be flexible, allowing adjustments for site-specific conditions if adequate information is available.
- To be appropriate for early-stage application, the methodology needs to be simple, requiring a minimum of site-specific data.
- The methodology should be consistent with current understanding of subsurface processes.
- The process of developing and applying SSLs should generate information that can be used and built upon as a site evaluation progresses.

Flexibility is achieved by using readily obtainable site-specific data in standardized equations; conservative default input parameters are also provided for use when site-specific data are not available. In addition, more complex unsaturated zone fate-and-transport models have been identified that can be used to calculate SSLs when more detailed site-specific information is available or can be obtained (see Part 3). These models can extend the applicability of SSLs to subsurface conditions that are not adequately addressed by the simple equations (e.g., deep water tables; clay layers or other unsaturated zone characteristics that can attenuate contaminants before they reach ground water).

The SSL methodology was designed for use during the early stages of a site evaluation when information about subsurface conditions may be limited. Because of this constraint, the methodology is based on conservative, simplifying assumptions about the release and transport of contaminants in the subsurface (see Highlight 2).

Highlight 2: Simplifying Assumptions for the Migration to Ground Water Pathway

- The source is infinite (i.e., steady-state concentrations will be maintained in ground water over the exposure period of interest).
- Contaminants are uniformly distributed throughout the zone of contamination.
- Soil contamination extends from the surface to the water table (i.e., adsorption sites are filled in the unsaturated zone beneath the area of contamination).
- There is no chemical or biological degradation in the unsaturated zone.
- Equilibrium soil/water partitioning is instantaneous and linear in the contaminated soil.
- The receptor well is at the edge of the source (i.e., there is no dilution from recharge downgradient of the site) and is screened within the plume.
- The aquifer is unconsolidated and unconfined (surficial).
- Aquifer properties are homogeneous and isotropic.
- There is no attenuation (i.e., adsorption or degradation) of contaminants in the aquifer.
- NAPLs are not present at the site.

Although simplified, the SSL methodology described in this section is theoretically and operationally consistent with the more sophisticated investigation and modeling efforts that are conducted to develop soil cleanup goals and cleanup levels for protection of ground water at Superfund sites. SSLs developed using this methodology can be viewed as evolving risk-based levels that can be refined as more site information becomes available. The early use of the methodology at a site will help focus further subsurface investigations on areas of true concern with respect to ground water quality and will provide information on soil characteristics, aquifer characteristics, and chemical properties that can be built upon as a site evaluation progresses.

2.5.1 Development of Soil/Water Partition Equation. The methodology used to estimate contaminant release in soil leachate is based on the Freundlich equation, which was developed to model sorption from liquids to solids. The basic Freundlich equation applied to the soil/water system is:

$$K_d = C_s / C_w^n \tag{11}$$

where

K_d = Freundlich soil/water partition coefficient (L/kg)
C_s = concentration sorbed on soil (mg/kg)
C_w = solution concentration (mg/L)
n = Freundlich exponent (dimensionless).

Assuming that adsorption is linear with respect to concentration (n=1)* and rearranging to backcalculate a sorbed concentration (C_s):

$$C_s = (K_d)\ C_w \tag{12}$$

For SSL calculation, C_w is the target soil leachate concentration.

Adjusting Sorbed Soil Concentrations to Total Concentrations. To develop a screening level for comparison with contaminated soil samples, the sorbed concentration derived above (C_s) must be related to the total concentration measured in a soil sample (C_t). In a soil sample, contaminants can be associated with the solid soil materials, the soil water, and the soil air as follows (Feenstra et al., 1991):

$$M_t = M_s + M_w + M_a \tag{13}$$

where

M_t = total contaminant mass in sample (mg)
M_s = contaminant mass sorbed on soil materials (mg)
M_w = contaminant mass in soil water (mg)
M_a = contaminant mass in soil air (mg).

Furthermore,

$$M_t = C_t\ \rho_b\ V_{sp}\ , \tag{14}$$

$$M_s = C_s\ \rho_b\ V_{sp}\ , \tag{15}$$

$$M_w = C_w\ \theta_w\ V_{sp}\ , \tag{16}$$

and

$$M_a = C_a\ \theta_a\ V_{sp}\ , \tag{17}$$

where

ρ_b = dry soil bulk density (kg/L)
V_{sp} = sample volume (L)
θ_w = water-filled porosity (L_{water}/L_{soil})
C_a = concentration on soil pore air (mg/L_{soil})
θ_a = air-filled soil porosity (L_{air}/L_{soil}).

For contaminated soils (with concentrations below C_{sat}), C_a may be determined from C_w and the dimensionless Henry's law constant (H') using the following relationship:

$$C_a = C_w\ H' \tag{18}$$

---

* The linear assumption will tend to overestimate sorption and underestimate desorption for most organics at higher concentrations (i.e., above 10^{-5} M for organics) (Piwoni and Banerjee, 1989).

thus

$$M_a = C_w H' \theta_a V_{sp} \qquad \textbf{(19)}$$

Substituting into Equation 13:

$$C_t = \frac{C_s\rho_b + C_w\theta_w + C_w H'\theta_a}{\rho_b} \qquad \textbf{(20)}$$

or

$$C_s = C_t - C_w \left(\frac{\theta_w + \theta_a H'}{\rho_b} \right) \qquad \textbf{(21)}$$

Substituting into Equation 12 and rearranging:

Soil-Water Partition Equation for Migration to Ground Water Pathway: Inorganic Contaminants

$$C_t = C_w \left(K_d + \frac{\theta_w + \theta_a H'}{\rho_b} \right) \qquad \textbf{(22)}$$

Parameter/Definition (units)	Default	Source
C_t/screening level in soil (mg/kg)	–	–
C_w/target soil leachate concentration (mg/L)	(nonzero MCLG, MCL, or HBL) × 20 DAF	Table 1 (nonzero MCLG, MCL); Section 2.5.6 (DAF for 0.5-acre source)
K_d/soil-water partition coefficient (L/kg)	chemical-specific	see Part 5
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.3 (30%)	U.S. EPA/ORD
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.13	$n - \theta_w$
n/total soil porosity (L_{pore}/L_{soil})	0.43	$1 - \rho_b/\rho_s$
ρ_b/dry soil bulk density (kg/L)	1.5	U.S. EPA, 1991b
ρ_s/soil particle density (kg/L)	2.65	U.S. EPA, 1991b
H'/dimensionless Henry's law constant	H × 41, where 41 is a conversion factor	U.S. EPA, 1991b
H/Henry's law constant (atm-m^3/mol)	chemical-specific	see Part 5

Equation 22 is used to calculate SSLs (total soil concentrations, C_t) corresponding to soil leachate concentrations (C_w) equal to the target contaminant soil leachate concentration. The equation assumes that soil water, solids, and gas are conserved during sampling. If soil gas is lost during sampling, θ_a should be assumed to be zero. Likewise, for inorganic contaminants except mercury, there is no significant vapor pressure and H' may be assumed to be zero.

The User's Guide (U.S. EPA, 1996) describes how to develop site-specific estimates of the soil parameters needed to calculate SSLs. Default soil parameter values for the partition equation are the same as those used for the VF equation (see Section 2.4.2) except for average water-filled soil porosity (θ_w). A conservative value (0.15) was used in the VF equation because the model is most sensitive to this parameter. Because migration to ground water SSLs are not particularly sensitive to soil water content (see Section 2.5.7), a value that is more typical of subsurface conditions (0.30) was used. This value is between the mean field capacity (0.20) of Class B soils (Carsel et al., 1988) and the saturated volumetric water content for loam (0.43).

K_d varies by chemical and soil type. Because of different influences on K_d values, derivations of K_d values for organic compounds and metals were treated separately in the SSL methodology.

2.5.2 Organic Compounds—Partition Theory. Past research has demonstrated that, for hydrophobic organic chemicals, soil organic matter is the dominant sorbing component in soil and that K_d is linear with respect to soil organic carbon content (OC) as long as OC is above a critical level (Dragun, 1988). Thus, K_d can be normalized with respect to soil organic carbon to K_{oc}, a chemical-specific partitioning coefficient that is independent of soil type, as follows:

$$K_d = K_{oc}\, f_{oc} \tag{23}$$

where

K_{oc} = organic carbon partition coefficient (L/kg)
f_{oc} = fraction of organic carbon in soil (mg/mg)

Substituting into Equation 22:

Soil-Water Partition Equation for Migration to Ground Water Pathway: Organic Contaminants

$$C_t = C_w \left((K_{oc}\, f_{oc}) + \frac{\theta_w + \theta_a H'}{\rho_b} \right) \tag{24}$$

Parameter/Definition (units)	Default	Source
C_t/screening level in soil mg/kg)	–	–
C_w/target leachate concentration (mg/L)	(nonzero MCLG, MCL, or HBL) × 20 DAF	Table 1 (MCL, nonzero MCLG); Section 2.5.6 (DAF for a 0.5-acre source)
K_{oc}/soil organic carbon-water partition coefficient (L/kg)	chemical-specific	see Part 5
f_{oc}/organic carbon content of soil (kg/kg)	0.002 (0.2%)	Carsel et al., 1988
θ_w/water-filled soil porosity (L_{water}/L_{soil})	0.3 (30%)	U.S. EPA/ORD
θ_a/air-filled soil porosity (L_{air}/L_{soil})	0.13	$n - \theta_w$
n/total soil porosity (L_{pore}/L_{soil})	0.43	$1 - \rho_b/\rho_s$
ρ_b/dry soil bulk density (kg/L)	1.5	U.S. EPA, 1991b
ρ_s/soil particle density (kg/L)	2.65	U.S. EPA, 1991b
H'/dimensionless Henry's law constant	H × 41, where 41 is a conversion factor	U.S. EPA, 1991b
H/Henry's law constant (atm-m^3/mol)	chemical-specific	see Part 5

Part 5 of this document provides K_{oc} values for organic chemicals and describes their development.

The critical organic carbon content, f_{oc}^* , represents OC below which sorption to mineral surfaces begins to be significant. This level is likely to be variable and to depend on both the properties of the soil and of the chemical sorbate (Curtis et al., 1986). Attempts to quantitatively relate f_{oc}^* to such properties have been made (see McCarty et al., 1981), but at this time there is no reliable method for estimating f_{oc}^* for specific chemicals and soils. Nevertheless, research has demonstrated that, for volatile halogenated hydrocarbons, f_{oc}^* is about 0.001, or 0.1 percent OC, for many low-carbon soils and aquifer materials (Piwoni and Banerjee, 1989; Schwarzenbach and Westall, 1981).

If soil OC is below this critical level, Equation 24 should be used with caution. This is especially true if soils contain significant quantities of fine-grained minerals with high sorptive properties (e.g., clays). If sorption to minerals is significant, Equation 24 will underpredict sorption and overpredict contaminant concentrations in soil pore water. However, this f_{oc}^* level is by no means the case for all soils; Abdul et al. (1987) found that, for certain organic compounds and aquifer materials, sorption was linear and could be adequately modeled down to $f_{oc} = 0.0003$ by considering K_{oc} alone.

For soils with significant inorganic and organic sorption (i.e., soils with $f_{oc} < 0.001$), the following equation has been developed (McCarty et al., 1981; Karickhoff, 1984):

$$K_d = (K_{oc}\, f_{oc}) + (K_{io}\, f_{io}) \tag{25}$$

where

K_{io} = soil inorganic partition coefficient
f_{io} = fraction of inorganic material
$f_{io} + f_{oc}$ = 1.

Although this equation is considered conceptually valid, K_{io} values are not available for the subject chemicals. Attempts to estimate K_{io} values by relating sorption on low-carbon materials to properties such as clay-size fraction, clay mineralogy, surface area, or iron-oxide content have not revealed any consistent correlations, and semiquantitative methods are probably years away (Piwoni and Banerjee, 1989). However, Piwoni and Banerjee developed the following empirical correlation (by linear regression, $r^2 = 0.85$) that can be used to estimate K_d values for hydrophobic organic chemicals from K_{ow} for low-carbon soils:

$$\log K_d = 1.01 \log K_{ow} - 0.36 \qquad \textbf{(26)}$$

where

K_{ow} = octanol/water partition coefficient.

The authors indicate that this equation should provide a K_d estimate that is within a factor of 2 or 3 of the actual value for nonpolar sorbates with $\log K_{ow} < 3.7$. This K_d estimate can be used in Equation 22 for soils with f_{oc} values less than 0.001. If sorption to inorganics is not considered for low-carbon soils where it is significant, Equation 24 will underpredict sorption and overpredict contaminant concentrations in soil pore water (i.e., it will provide a conservative estimate).

The use of fixed K_{oc} values in Equation 24 is valid only for hydrophobic, nonionizing organic chemicals. Several of the organic chemicals of concern ionize in the soil environment, existing in both neutral and ionized forms within the normal soil pH range. The relative amounts of the ionized and neutral species are a function of pH. Because the sorptive properties of these two forms differ, it is important to consider the relative amounts of the neutral and ionized species when determining K_{oc} values at a particular pH. Lee et al. (1990) developed a theoretically based algorithm, developed from thermodynamic equilibrium equations, and demonstrated that the equation adequately predicts laboratory-measured K_{oc} values for pentachlorophenol (PCP) and other ionizing organic acids as a function of pH.

The equation assumes that sorbent organic carbon determines the extent of sorption for both the ionized and neutral species and predicts the overall sorption of a weak organic acid ($K_{oc,p}$) as follows:

$$K_{oc,p} = K_{oc,n}\,\Phi_n + K_{oc,i}\,(1 - \Phi_n) \qquad \textbf{(27)}$$

where

$K_{oc,n}$, $K_{oc,i}$ = sorption coefficients for the neutral and ionized species (L/kg)
Φ_n = $(1 + 10^{pH - pKa})^{-1}$
pKa = acid dissociation constant.

This equation was used to develop K_{oc} values for ionizing organic acids as a function of pH, as described in Part 5. The User’s Guide (U.S. EPA, 1996) provides guidance on conducting site-specific measurements of soil pH for estimating K_{oc} values for ionizing organic compounds. Because a national distribution of soil pH values is not available, a median U.S. ground water pH (6.8) from the STORET database (U.S. EPA, 1992a) is used as a default soil pH value that is representative of subsurface pH conditions.

2.5.3 Inorganics (Metals)—Partition Theory. Equation 22 is used to estimate SSLs for metals for the migration to ground water pathway. The derivation of K_d values is much more complicated for metals than for organic compounds. Unlike organic compounds, for which K_d values are largely controlled by a single parameter (soil organic carbon), K_d values for metals are significantly affected by a variety of soil conditions. The most significant parameters are pH, oxidation-reduction conditions, iron oxide content, soil organic matter content, cation exchange capacity, and major ion chemistry. The number of significant influencing parameters, their variability in the field, and differences in experimental methods result in a wide range of K_d values for individual metals reported in the literature (over 5 orders of magnitude). Thus, it is much more difficult to derive generic K_d values for metals than for organics.

The K_d values used to generate SSLs for Ag, Ba, Be, Cd, Cr^{+3}, Cu, Hg, Ni, and Zn were developed using an equilibrium geochemical speciation model (MINTEQ2). The values for As, Cr^{6+}, Se, and Th were taken from empirical, pH-dependent adsorption relationships developed by EPA/ORD. Metal K_d values for SSL application are presented in Part 5, along with a description of their development and limitations. As with the ionizing organics, K_d values are selected as a function of site-specific soil pH, and metal K_d values corresponding to a pH of 6.8 are used as defaults where site-specific pH measurements are not available.

2.5.4 Assumptions for Soil/Water Partition Theory. The following assumptions are implicit in the SSL partitioning methodology. *These assumptions and their implications for SSL accuracy should be read and understood before using this methodology to calculate SSLs.*

1. **There is no contaminant loss due to volatilization or degradation.** The source is considered to be infinite; i.e., these processes do not reduce soil leachate concentrations over time. This is a **conservative** assumption, especially for smaller sites.

2. **Adsorption is linear with concentration.** The methodology assumes that adsorption is independent of concentration (i.e., the Freundlich exponent = 1). This has been reported to be true for various halogenated hydrocarbons, polynuclear aromatic hydrocarbons, benzene, and chlorinated benzenes. In addition, this assumption is valid at low concentrations (e.g., at levels close to the MCL) for most chemicals. As concentrations increase, however, the adsorption isotherm can depart from the linear.

   Studies on trichloroethane (TCE) and chlorobenzene indicate that departure from linear is in the **nonconservative** direction, with adsorbed concentrations being lower than predicted by a linear isotherm. However, adequate information is not available to establish nonlinear adsorption isotherms for the chemicals of interest. Furthermore, since the SSLs are derived at relatively low target soil leachate concentrations, departures from the linear at high concentrations do not significantly influence the accuracy of the results.

3. **The system is at equilibrium with respect to adsorption.** This ignores adsorption/desorption kinetics by assuming that the soil and pore water concentrations are at equilibrium levels. In other words, the pore-water residence time is assumed to be longer than the time it takes for the system to reach equilibrium conditions.

   This assumption is **conservative**. If equilibrium conditions are not met, the concentration in the pore water will be less than that predicted by the methodology. The kinetics of adsorption are not adequately understood for a sufficient number of chemicals and site conditions to consider equilibrium kinetics in the methodology.

4. **Adsorption is reversible.** The methodology assumes that desorption processes operate in the same way as adsorption processes, since most of the K_{oc} values are measured by adsorption experiments rather than by desorption experiments. In actuality, desorption is slower to some degree than adsorption and, in some cases, organics can be irreversibly bound to the soil matrix. In general, the significance of this effect increases with K_{ow}.

   This assumption is **conservative**. Slower desorption rates and irreversible sorption will result in lower pore-water concentrations than that predicted by the methodology. Again, the level of knowledge on desorption processes is not sufficient to consider desorption kinetics and degree of reversibility for all of the subject chemicals.

2.5.5 Dilution/Attenuation Factor Development. As contaminants in soil leachate move through soil and ground water, they are subjected to physical, chemical, and biological processes that tend to reduce the eventual contaminant concentration at the receptor point (i.e., drinking water well). These processes include adsorption onto soil and aquifer media, chemical transformation (e.g., hydrolysis, precipitation), biological degradation, and dilution due to mixing of the leachate with ambient ground water. The reduction in concentration can be expressed succinctly by a DAF, which is defined as the ratio of contaminant concentration in soil leachate to the concentration in ground water at the receptor point. When calculating SSLs, a DAF is used to backcalculate the target soil leachate concentration from an acceptable ground water concentration (e.g., MCLG). For example, if the acceptable ground water concentration is 0.05 mg/L and the DAF is 10, the target leachate concentration would be 0.5 mg/L.

The SSL methodology addresses only one of these dilution-attenuation processes: contaminant dilution in ground water. A simple equation derived from a geohydrologic water-balance relationship has been developed for the methodology, as described in the following subsection. The ratio factor calculated by this equation is referred to as a dilution factor rather than a DAF because it does not consider processes that attenuate contaminants in the subsurface (i.e., adsorption and degradation processes). This simplifying assumption was necessary for several reasons.

First, the infinite source assumption results in all subsurface adsorption sites being eventually filled and no longer available to attenuate contaminants. Second, soil contamination extends to the water table, eliminating attenuation processes in the unsaturated zone. Additionally, the receptor well is assumed to be at the edge of the source, minimizing the opportunity for attenuation in the aquifer. Finally, chemical-specific biological and chemical degradation rates are not known for many of the SSL chemicals; where they are available they are usually based on laboratory studies under simplified, controlled conditions. Because natural subsurface conditions such as pH, redox conditions, soil mineralogy, and available nutrients have been shown to markedly affect natural chemical and biological degradation rates, and because the national variability in these properties is significant and has not been characterized, EPA does not believe that it is possible at this time to incorporate these degradation processes into the simple site-specific methodology for national application.

If adsorption or degradation processes are expected to significantly attenuate contaminant concentrations at a site (e.g., for sites with deep water tables or soil conditions that will attenuate contaminants), the site manager is encouraged to consider the option of using more sophisticated fate and transport models. Many of these models can consider adsorption and degradation processes and can model transient conditions necessary to consider a finite source size. Part 3 of this document presents information on the selection and use of such models for SSL application.

The dilution factor model assumes that the aquifer is unconfined and unconsolidated and has homogeneous and isotropic properties. Unconfined (surficial) aquifers are common across the country, are vulnerable to contamination, and can be used as drinking water sources by local residents. Dilution model results may not be applicable to fractured rock or karst aquifer types. The site manager should consider use of more appropriate models to calculate a dilution factor (or DAF) for such settings.

In addition, the simple dilution model does not consider facilitated transport. This ignores processes such as colloidal transport, transport via solvents other than water (e.g., NAPLs), and transport via dissolved organic matter (DOM). These processes have greater impact as K_{ow} (and hence, K_{oc}) increases. However, the transport via solvents other than water is operative only if certain site-specific conditions are present. Transport by DOM and colloids has been shown to be potentially significant under certain conditions in laboratory and field studies. Although much research is in progress on these processes, the current state of knowledge is not adequate to allow for their consideration in SSL calculations.

If there is the potential for the presence of NAPLs in soils at the site or site area in question, SSLs should not be used for this area (i.e., further investigation is required). The C_{sat} equation (Equation 9) presented in Section 2.4.4 can be used to estimate the contaminant concentration at which the presence of pure-phase NAPLs may be suspected for contaminants that are liquid at soil temperature. If NAPLs are suspected in site soils, refer to U.S. EPA (1992c) for additional guidance on how to estimate the potential for DNAPL occurrence in the subsurface.

Dilution Model Development. EPA evaluated four simple water balance models to adjust SSLs for dilution in the aquifer. Although written in different terms, all four options reviewed can be expressed as the same simple water balance equation to calculate a dilution factor, as follows:

Option 1 (ASTM):

$$\text{dilution factor} = (1 + U_{gw}\, d/IL) \qquad \textbf{(28)}$$

where

U_{gw} = Darcy ground water velocity (m/yr)
d = mixing zone depth (m)
I = infiltration rate (m/yr)
L = length of source parallel to flow (m).

For Darcy velocity:

$$U_{gw} = Ki \qquad \textbf{(29)}$$

where

K = aquifer hydraulic conductivity (m/yr)
i = hydraulic gradient (m/m).

Thus

$$\text{dilution factor} = 1 + (Kid/IL) \qquad \textbf{(30)}$$

Option 2 (EPA Ground Water Forum):

$$\text{dilution factor} = (Q_p + Q_A)/Q_p \qquad \textbf{(31)}$$

where

Q_p = percolation flow rate (m^3/yr)
Q_A = aquifer flow rate (m^3/yr)

For percolation flow rate:

$$Q_p = IA \qquad \textbf{(32)}$$

where

A = facility area (m^2) = WL.

For aquifer flow rate:

$$Q_A = WdKi \qquad \textbf{(33)}$$

where

W = width of source perpendicular to flow (m)
d = mixing zone depth (m).

Thus

$$\text{dilution factor} = (IA + WdKi)/IWL$$

$$= 1 + (Kid/IL) \qquad \textbf{(34)}$$

Option 3 (Summers Model):

$$C_w = (Q_p\, C_p)/(Q_p + Q_A) \qquad \textbf{(35)}$$

where

C_w = ground water contaminant concentration (mg/L)
C_p = soil leachate concentration (mg/L)

given that

$$C_w = C_p/\text{dilution factor}$$

$$1/\text{dilution factor} = Q_p/(Q_p + Q_A)$$

or

$$\text{dilution factor} = (Q_p + Q_A)/Q_p \text{ (see } \textbf{Option 2}\text{)}$$

Option 4 (EPA ORD/RSKERL):

$$\text{dilution factor} = (Q_p + Q_A)/Q_p = RX/RL \qquad \textbf{(36)}$$

where

R = recharge rate (m/yr) = infiltration rate (I, m/yr)
X = distance from receptor well to ground water divide (m)

(Note that the intermediate equation is the same as **Option 2**.)

This option is a longer-term option that is not considered further in this analysis because valid X values are not currently available either nationally or for specific sites. EPA is considering developing regional estimates for these parameters.

Dilution Model Input Parameters. As shown, all three options for calculating contaminant dilution in ground water can be expressed as the same equation:

Ground Water Dilution Factor

$$\text{dilution factor} = 1 + (Kid/IL) \qquad \textbf{(37)}$$

Parameter/Definition (units)
K/aquifer hydraulic conductivity (m/yr)
i/hydraulic gradient (m/m)
d/mixing zone depth (m)
I/infiltration rate (m/yr)
L/source length parallel to ground water flow (m)

Mixing Zone Depth (**d**). Because of its dependence on the other variables, mixing zone depth is estimated with the method used for the MULTIMED model (Sharp-Hansen et al., 1990). The MULTIMED estimation method was selected to be consistent with that used by EPA's Office of Solid Waste for the EPA Composite Model for Landfills (EPACML). The equation for estimating mixing zone depth (d) is as follows:

$$d = (2\alpha_v L)^{0.5} + d_a \{1 - \exp[(-LI)/(V_s n_e d_a)]\} \qquad \textbf{(38)}$$

where

α_v = vertical dispersivity (m/m)
V_s = horizontal seepage velocity (m/yr)
n_e = effective aquifer porosity ($L_{pore}/L_{aquifer}$)
d_a = aquifer depth (m).

The first term, $(2\alpha_v L)^{0.5}$, estimates the depth of mixing due to vertical dispersivity ($d_{\alpha v}$) along the length of ground water travel. Defining the point of compliance with ground water standards at the downgradient edge of the source, this travel distance becomes the length of the source parallel to flow L. Vertical dispersivity can be estimated by the following relationship (Gelhar and Axness, 1981):

$$\alpha_v = 0.056\ \alpha_L \qquad \textbf{(39)}$$

where

α_L = longitudinal dispersivity = 0.1 x_r
x_r = horizontal distance to receptor (m).

Because the potential receptor is assumed to have a well at the edge of the facility, $x_r = L$ and

$$\alpha_v = 0.0056\ L \qquad \textbf{(40)}$$

Thus

$$d_{\alpha v} = (0.0112\ L^2)^{0.5} \qquad \textbf{(41)}$$

The second term, $d_a\ \{1 - \exp[(-LI) / (V_s n_e d_a)]\}$, estimates the depth of mixing due to the downward velocity of infiltrating water, d_{Iv}. In this equation, the following substitution may be made:

$$V_s = Ki/n_e \qquad \textbf{(42)}$$

so

$$d_{Iv} = d_a\ \{1 - \exp[(-LI)/(Kid_a)]\} \qquad \textbf{(43)}$$

Thus, mixing zone depth is calculated as follows:

$$d = d_{\alpha v} + d_{Iv} \qquad \textbf{(44)}$$

Estimation of Mixing Zone Depth

$$d = (0.0112\ L^2)^{0.5} + d_a\ \{1 - \exp[(-LI)/(Kid_a)]\} \qquad \textbf{(45)}$$

Parameter/Definition (units)
d/mixing zone depth (m)
L/source length parallel to ground water flow (m)
I/infiltration rate (m/yr)
K/aquifer hydraulic conductivity (m/yr)
d_a/aquifer thickness (m)

Incorporation of this equation for mixing zone depth into the SSL dilution equation results in five parameters that must be estimated to calculate dilution: source length (L), infiltration rate (I), aquifer hydraulic conductivity (K), aquifer hydraulic gradient (i), and aquifer thickness (d_a). Aquifer thickness also serves as a limit for mixing zone depth. The User's Guide (U.S. EPA, 1996) describes how to develop site-specific estimates for these parameters. Parameter definitions and defaults used to develop generic SSLs are as follows:

- **Source Length (L)** is the length of the source (i.e., area of contaminated soil) parallel to ground water flow and affects the flux of contaminant released in soil leachate (IL) as well as the depth of mixing in the aquifer. The default option for this parameter assumes a square, 0.5-acre contaminant source. This default was changed from 30 acres in response to comments to be more representative of actual contaminated soil sources (see Section 1.3.4). Increasing source area (and thereby area) may result in a lower dilution factor. Appendix A includes an analysis of the conservatism associated with the 0.5-acre source size.

- **Infiltration Rate (I)**. Infiltration rate times the source area determines the amount of contaminant (in soil leachate) that enters the aquifer over time. Thus, increasing infiltration decreases the dilution factor. Two options can be used to generate infiltration rate estimates for SSL calculation. The first assumes that infiltration rate is equivalent to recharge. This is generally true for uncontrolled contaminated soil sites but would be conservative for capped sites (infiltration < recharge) and nonconservative for sites with an additional source of infiltration, such as surface impoundments (infiltration > recharge). Recharge estimates for this option can be obtained from Aller et al. (1987) by hydrogeologic setting, as described in Section 2.5.6.

  The second option is to use the HELP model to estimate infiltration, as was done for OSW's EPACML and EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) modeling efforts. The Soil Screening Guidance (U.S. EPA, 1995c) provides information on obtaining and using the HELP model to estimate site-specific infiltration rates.

- **Aquifer Parameters**. Aquifer parameters needed for the dilution factor model include hydraulic conductivity (K, m/yr), hydraulic gradient (i, m/m), and aquifer thickness (d_a, m). The User's Guide (U.S. EPA, 1996) describes how to develop aquifer parameter estimates for calculating a site-specific dilution factor.

2.5.6 Default Dilution-Attenuation Factor.

EPA has selected a default DAF of 20 to account for contaminant dilution and attenuation during transport through the saturated zone to a compliance point (i.e., receptor well). At most sites, this adjustment will more accurately reflect a contaminant's threat to ground water resources than assuming a DAF of 1 (i.e., no dilution or attenuation). EPA selected a DAF of 20 using a "weight of evidence" approach. This approach considers results from OSW's EPACMTP model as well as results from applying the SSL dilution model described in Section 2.5.5 to 300 ground water sites across the country.

The default DAF of 20 represents an adjustment from the DAF of 10 presented in the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h) to reflect a change in default source size from 30 acres to 0.05 acre. A DAF of 20 is protective for sources up to 0.5 acre in size. Analyses presented in Appendix A indicate that it can be protective of larger sources as well. However, this hypothesis should be examined on a case-by-case basis before applying a DAF of 20 to sources larger than 0.5 acre.

EPACMTP Modeling Effort. One model considered during selection of the default DAF is described in *Background Document for EPA's Composite Model for Leachate Migration with Transformation Products* (U.S. EPA, 1993a). EPACMTP has a three-dimensional module to simulate ground water flow that can account for mounding under waste sites. The model also has a three-dimensional transport module and both linear and nonlinear adsorption in the unsaturated and saturated zones and can simulate chain decay, thus allowing the simulation of the formation and the fate and transport of daughter (transformation) products of degrading chemicals. The model can also be used to simulate a finite source scenario.

EPACMTP is comprised of three main interconnected modules:

- An unsaturated zone flow and contaminant fate and transport module
- A saturated zone ground water flow and contaminant fate and transport module
- A Monte Carlo driver module, which generates model parameters from nationwide probability distributions.

The unsaturated and saturated zone modules simulate the migration of contaminants from initial release from the soil to a downgradient receptor well. More information on the EPACMTP model is provided in Appendix E.

EPA has extensively verified both the unsaturated and saturated zone modules of the EPACMTP against other available analytical and numerical models to ensure accuracy and efficiency. Both the unsaturated zone and the saturated zone modules of the EPACMTP have been reviewed by the EPA Science Advisory Board and found to be suitable for generic applications such as the derivation of nationwide DAFs.

EPACMTP Model Inputs (SSL Application). For nationwide Monte Carlo model applications, the input to the model is in the form of probability distributions of each of the model input parameters. The output from the model consists of the probability distribution of DAF values, representing the likelihood that the DAF will not be less than a certain value. For instance, a 90th percentile DAF of 10 means that the DAF will be 10 or higher in at least 90 percent of the cases.

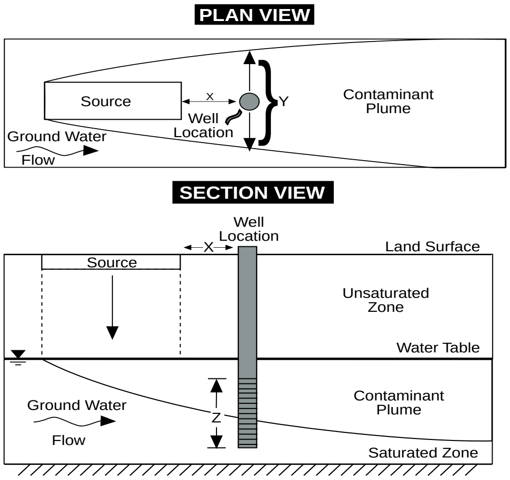
For each model input parameter, a probability distribution is provided, describing the nationwide likelihood that the parameter has a certain value. The parameters are divided into four main groups:

- Source-specific parameters, e.g., area of the waste unit, infiltration rate
- Chemical-specific parameters, e.g., hydrolysis constants, organic carbon partition coefficient

- Unsaturated zone-specific parameters, e.g., depth to water table, soil hydraulic conductivity

- Saturated zone-specific parameters, e.g., saturated zone thickness, ambient ground water flow rate, location of nearest receptor well.

Probability distributions for each parameter used in the model have been derived from nationwide surveys of waste sites, such as EPA's landfill survey (53 FR 28692). During the Monte Carlo simulation, values for each model parameter are randomly drawn from their respective probability distributions. In the calculation of the DAFs for generic SSLs, site data from over 1,300 municipal landfill sites in OSW's Subtitle D Landfill Survey were used to define parameter ranges and distributions. Each combination of randomly drawn parameter values represents one out of a practically infinite universe of possible waste sites. The fate and transport modules are executed for the specific set of model parameters, yielding a corresponding DAF value. This procedure is repeated, typically on the order of several thousand times, to ensure that the entire universe of possible parameter combinations (waste sites) is adequately sampled. In the derivation of DAFs for generic SSLs, the model simulations were repeated 15,000 times for each scenario investigated. At the conclusion of the analysis, a cumulative frequency distribution of DAF values was constructed and plotted.



Parameters:

- X (distance from source to well) = 0 ft
- Y (transverse well location) = Monte Carlo within 1/2 width of source
- Z (well intake point below water table) = Monte Carlo, range 15 → 300 ft
- Rainfall = Monte Carlo
- Soil type = Monte Carlo
- Depth to aquifer = Monte Carlo
- Assumes infinite source term

Figure 3. Migration to ground water pathway—EPACMTP modeling effort.

EPA assumed an infinite waste source of fixed area for the generic SSL modeling scenario. EPA chose this relatively conservative assumption because of limited information on the nationwide distribution of the volumes of contaminated soil sources. For the SSL modeling scenario, EPA performed a number of sensitivity analyses consisting of fixing one parameter at a time to determine the parameters that have the greatest impact on DAFs. The results of the sensitivity analyses indicate that the climate (net precipitation), soil types, and size of the contaminated area have the greatest effect on the DAFs. The EPA feels that the size of the contaminated area lends itself most readily to practical application to SSLs.

To calculate DAFs for the SSL scenario, the receptor point was taken to be a domestic drinking water well located on the downgradient edge of the contaminated area. The location of the intake point (receptor well screen) was assumed to vary between 15 and 300 feet below the water table (these values are based on empirical data reflecting a national sample distribution of depth of residential drinking water wells). The location of the intake point allows for mixing within the aquifer. EPA believes that this is a reasonable assumption because there will always be some dilution attributed to the pumping of water for residential use from an aquifer. The horizontal placement of the well was assumed to vary uniformly along the center of the downgradient edge of the source within a width of one-half of the width of the source. Degradation and retardation of contaminants were not considered in this analysis. Figure 3 is a schematic showing aspects of the subsurface SSL conceptual model used in the EPACMTP modeling effort. Appendix E is the background document prepared by EPA/OSW for this modeling effort.

EPACMTP Model Results. The results of the EPACMTP analyses indicate a DAF of about 170 for a 0.5-acre source at the 90th percentile protection level (Table 5). If a 95th percentile protection level is used, a DAF of 7 is protective for a 0.5-acre source.

Table 5. Variation of DAF with Size of Source Area for SSL EPACMTP Modeling Effort

	DAF		
Area (acres)	85th	90th	95th
0.02	1.42E+07	2.09E+05	946
0.04	9.19E+05	2.83E+04	211
0.11	5.54E+04	2.74E+03	44
0.23	1.16E+04	644	15
0.50	2.50E+03	170	7.0
0.69	1.43E+03	120	4.5
1.1	668	60	3.1
1.6	417	38	2.5
1.8	350	33	2.3
3.4	159	18	1.7
4.6	115	13	1.6
11.5	41	5.5	1.2
23	21	3.5	1.2
30	16	3.0	1.1
46	12	2.4	1.1
69	8.7	2.0	1.1

Dilution Factor Modeling Effort. To gain further information on the national range and distribution of DAF values, EPA also applied the simple SSL water balance dilution model to ground water sites included in two large surveys of hydrogeologic site investigations. These were American Petroleum Institute's (API's) hydrogeologic database (HGDB) and EPA's database of conditions at Superfund sites contaminated with DNAPL.

The HGDB contains the results of a survey sponsored by API and the National Water Well Association (NWWA) to determine the national variability in simple hydrogeologic parameters (Newell et al., 1989). The survey was conducted to validate EPA's use of the EPACML model as a screening tool for the land disposal of hazardous wastes. The survey involved more than 400 ground water professionals who submitted data on aquifer characteristics from field investigations at actual waste sites and other ground water projects. The information was compiled in HGDB, which is available from API and is included in OASIS, an EPA-sponsored ground water decision support system. Newell et al. (1990) also present these data as "national average" conditions and by hydrogeologic settings based on those defined by Aller et al. (1987) for the DRASTIC modeling effort. Aller et al. (1987) defined these settings within the overall framework defined by Heath's ground water regions (Heath, 1984). The HGDB estimates of hydraulic conductivity and hydraulic gradient show reasonable agreement with those in Aller et al. (1987), which serves as another source of estimates for these parameters.

The SSL dilution factor model (including the associated mixing zone depth model) requires estimates for five parameters:

d_a = aquifer thickness (m)
L = length of source parallel to flow (m)
I = infiltration rate (m/yr)
K = aquifer hydraulic conductivity (m/yr)
i = hydraulic gradient (m/m).

Dilution factors were calculated by individual HGDB or DNAPL site to retain as much site-correlated parameter information as possible. The HGDB contains estimates of aquifer thickness (d_a), aquifer hydraulic conductivity (K), and aquifer hydraulic gradient (i) for 272 ground water sites. The aquifer hydraulic conductivity estimates were examined for these sites, and sites with reported values less than 5×10^{-5} cm/s were culled from the database because formations with lower hydraulic conductivity values are not likely to be used as drinking water sources. In addition, sites in fractured rock or solution limestone settings were removed because the dilution factor model does not adequately address such aquifers. This resulted in 208 sites remaining in the HGDB. The DNAPL site database contains 92 site estimates of seepage velocity ($\bar{v}$), which can be related to hydraulic conductivity and hydraulic gradient by the following relationship:

$$\bar{v} = Ki / n_e \tag{46}$$

where

n_e = effective porosity.

Effective porosity (n_e) was assumed to be 0.35, which is representative of sand and gravel aquifers (the most prevalent aquifer type in the HGDB). Thus, for the DNAPL sites, $0.35 \times \bar{v}$ was substituted for Ki in the dilution factor equation.

Estimates of the other parameters required for the modeling effort are described below. Site-specific values were used where available. Because the modeling effort uses a number of site-specific modeling results to determine a nationwide distribution of dilution factors, typical values were used to estimate parameters for sites without site-specific estimates.

Source Length (L). The contaminant source (i.e., area of soil contamination) was assumed to be square. This assumption may be conservative for sites with their longer dimensions perpendicular to ground water flow or nonconservative for sites with their longer dimensions parallel to ground water flow. The source length was calculated as the square root of the source area for the source sizes in question. To cover a range of contaminated soil source area sizes, five source sizes were modeled: 0.5 acre, 10 acres, 30 acres, 60 acres, and 100 acres.

Infiltration Rate (I). Infiltration rate estimates were not available in either database. Recharge estimates for individual hydrogeologic settings from Aller et al. (1987) were used as infiltration estimates (i.e., it was assumed that infiltration = recharge). Because of differences in database contents, it was necessary to use different approaches to obtaining recharge/infiltration estimates for the HGDB and DNAPL sites.

The HGDB places each of its sites in one of the hydrogeologic settings defined by Aller et al. (1987). A recharge estimate for each HGDB site was simply extracted for the appropriate setting from Aller et al. The median of the recharge range presented was used (Table 6).

The DNAPL database does not contain sufficient hydrogeologic information to place each site into the Aller et al. settings. Instead, each of the 92 DNAPL sites was placed in one of Heath's ground water regions. The sites were found to lie within five hydrogeologic regions: nonglaciated central, glaciated central, piedmont/blue ridge, northeast and superior uplands, and Atlantic/Gulf coastal plain. Recharge was estimated for each region by averaging the median recharge value from all hydrogeologic settings except for those with steep slopes. The appropriate Heath region recharge estimate was then used for each DNAPL site in the dilution factor calculations.

Aquifer Parameters. All aquifer parameters needed for the SSL dilution model are included in the HGDB. Because hydraulic conductivity and gradient are included in the seepage velocity estimates in the DNAPL site database, only aquifer thickness was unknown for these sites. Aquifer thickness for all DNAPL sites was set at 9.1 m, which is the median value for the "national average" condition in the HGDB (Newell et al., 1990).

Dilution Modeling Results. Table 7 presents summary statistics for the 92 DNAPL sites, the 208 HGDB sites, and all 300 sites. One can see that the HGDB sites generally have lower dilution factors than the DNAPL sites, although the absolute range in values is greater in the HGDB. However, the available information for these sites is insufficient to fully explain the differences in these data sets. The wide range of dilution factors for these sites reflects the nationwide variability in hydrogeologic conditions affecting this parameter. The large difference between the average and geometric mean statistics indicates a distribution skewed toward the lower dilution factor values. The geometric mean represents a better estimate of the central tendency of such skewed distributions. Appendix F presents the dilution modeling inputs and results for the HGDB and DNAPL sites, tabulated by individual site.

Selection of the Default DAF. The default DAF was selected considering the evidence of the national DAF and dilution factor estimates described above. A DAF of 10 was selected in the December 1994 draft Soil Screening Guidance to be protective of a 30-acre source size. The EPACMTP model results showed a DAF of 3 for 30 acres at the 90th percentile. The SSL dilution model results have geometric mean dilution factors for a 30-acre source of 10 and 7 for DNAPL sites and HGDB sites, respectively. In a weight of evidence approach, more weight was given to the results of the DNAPL sites because they are representative of the kind of sites to which SSLs are likely to be applied. Considering the conservative assumptions in the SSL dilution factor model (see Section 2.5.5), and the conservatism inherent in the soil partition methodology (see Section 2.5.4), EPA believes (1) that these results support the use of a DAF of 10 for a 30-acre source, and (2) that this DAF will protect human health from exposure through this pathway at most Superfund sites across the Nation

Table 6. Recharge Estimates for DNAPL Site Hydrogeologic Regions

	Recharge (m/yr)		
Hydrogeologic setting	**Min.**	**Max.**	**Avg.**
Nonglaciated Central (Region 6)			
Alluvial Mountain Valleys	0.10	0.18	0.14
Alter. SS/LS/Sh., Thin Soil	0.10	0.18	0.14
Alter. SS/LS/Sh., Deep Regolith	0.10	0.18	0.14
Solution Limestone*	0.25	0.38	0.32
Alluvium w/ Overbank Deposits	0.18	0.25	0.22
Alluvium w/o Overbank Deposits	0.18	0.25	0.22
Braided River Deposits	0.10	0.18	0.14
Triassic Basins	0.10	0.18	0.14
Swamp/Marsh	0.10	0.18	0.14
Met./Ig. Domes & Fault Blocks	0.00	0.05	0.03
Unconsol./Semiconsol. Aquifers	0.00	0.05	0.03
	Overall Average:		*0.15*
Glaciated Central (Region 7)			
Glacial Till Over Bedded Rock	0.10	0.18	0.14
Glacial Till Over Outwash	0.10	0.18	0.14
Glacial Till Over Sol. Limestone	0.10	0.18	0.14
Glacial Till Over Sandstone	0.10	0.18	0.14
Glacial Till Over Shale	0.10	0.18	0.14
Outwash	0.18	0.25	0.22
Outwash Over Bedded Rock*	0.25	0.38	0.32
Outwash Over Solution Limestone*	0.25	0.38	0.32
Moraine	0.18	0.25	0.22
Buried Valley	0.18	0.25	0.22
Alluvium w/ Overbank Deposits	0.10	0.18	0.14
Alluvium w/o Overbank Deposits*	0.25	0.38	0.32
Glacial Lake Deposits	0.10	0.18	0.14
Thin Till Over Bedded Rock	0.18	0.25	0.22
Beaches, B. Ridges, Dunes*	0.25	0.38	0.32
Swamp/Marsh	0.10	0.18	0.14
	Overall Average:		*0.20*
Piedmont/Blue Ridge (Region 8)			
Alluvial Mountain Valleys	0.18	0.25	0.22
Regolith	0.10	0.18	0.14
River Alluvium	0.18	0.25	0.22
Mountain Crests	0.00	0.05	0.03
Swamp/Marsh	0.10	0.18	0.14
	Overall Average:		*0.15*
Northeast & Superior Uplands (Region 9)			
Alluvial Mountain Valleys	0.18	0.25	0.22
Till Over Crystalline Bedrock	0.18	0.25	0.22
Glacial Till Over Outwash	0.18	0.25	0.22
Outwash*	0.25	0.38	0.32
Moraine	0.18	0.25	0.22
Alluvium w/ Overbank Deposits	0.18	0.25	0.22
Alluvium w/o Overbank Deposits*	0.25	0.38	0.32
Swamp/Marsh	0.10	0.18	0.14
Bedrock Uplands	0.10	0.18	0.14
Glacial Lake/Marine Deposits	0.10	0.18	0.14
Beaches, B. Ridges, Dunes*	0.25	0.38	0.32
	Overall Average:		*0.22*
Atlantic/Gulf Coastal Plain (Region 10)			
Regional Aquifers	0.00	0.05	0.03
Un./Semiconsol. Surficial Aquifer*	0.25	0.38	0.32
Alluvium w/ Overbank Deposits	0.18	0.25	0.22
Alluvium w/o Overbank Deposits*	0.25	0.38	0.32
Swamp*	0.25	0.38	0.32
	Overall Average:		*0.24*

Source: Aller et al. (1987); hydrogeologic regions from Heath (1984).

** 0.25 m to 0.38 m (9.8 in to 15 in) used as recharge range for 25+ m setting values from Aller et al. (1987).*

Table 7. SSL Dilution Factor Model Results: DNAPL and HGDB Sites

	Source area (acres)				
	0.5	**10**	**30**	**100**	**600**
DNAPL Sites (92)					
Geomean	34	15	10	6	4
Average	321	138	80	44	19
10th percentile	3	2	1	1	1
25th percentile	8	4	3	2	1
Median	30	13	8	5	3
75th percentile	140	60	35	20	9
90th percentile	336	144	84	46	20
HGDB sites (208)					
Geomean	16	10	7	5	3
Average	958	829	561	371	159
10th percentile	2	1	1	1	1
25th percentile	3	2	1	1	1
Median	10	6	5	3	2
75th percentile	56	30	19	12	5
90th percentile	240	134	90	51	21
All 300 sites					
Geomean	20	11	8	6	3
Average	763	617	414	271	116
10th percentile	2	1	1	1	1
25th percentile	4	2	2	1	1
Median	15	8	5	4	2
75th percentile	70	35	23	13	6
90th percentile	292	144	88	49	21

DNAPL = DNAPL Site Survey (EPA/OERR).
HGDB = Hydrogeologic database (API).

To adjust the 30-acre DAF for a 0.5-acre source, EPA considered the geomean 0.5-acre dilution factors for the DNAPL sites (34), HGDB sites (16), and all 300 sites (20). A default DAF of 20 was selected as a conservative value for a 0.5-acre source size.

This value also reflects the ratio between 0.5-acre and 30-acre geomean and median dilution factors calculated for the HGDB sites (2.2 and 2.0, respectively). The HGDB data reflect the influence of source size on actual dilution factors more accurately than the DNAPL site data because the HGDB includes site-specific estimates of aquifer thickness. As shown in the following section, aquifer thickness has a strong influence on the effect of source size on the dilution factor since it provides an upper limit on mixing zone depth. Increasing source area increases infiltration, which lowers the dilution factor, but also increases mixing zone depth, which increases the dilution factor. For an infinitely thick aquifer, these effects tend to cancel each other, resulting in similar dilution factors for 0.5 and 30 acres. Thin aquifers limit mixing depth for larger sources; thus the added infiltration predominates and lowers the dilution factors for the larger source. Since the DNAPL dilution factor analyses use a fixed aquifer depth, they tend to overestimate the reduction in dilution factors that result from a smaller source.

2.5.7 Sensitivity Analysis. A sensitivity analysis was conducted to examine the effects of site-specific parameters on migration to ground water SSLs. Both the partition equation and the dilution factor model were considered in this analysis. Because an adequate database of national distributions of these parameters was not available, a nominal range method was used to conduct the analysis. In this analysis, independent parameters were selected and each was taken to maximum and minimum values while keeping all other parameters at their nominal, or default, values.

Overall, SSLs are most sensitive to changes in the dilution factor. As shown in Table 7, the 10th to 90th percentile dilution factors vary from 2 to 292 for the 300 DNAPL and HGDB sites. Much of this variability can be attributed to the wide range of aquifer hydraulic conductivity across the Nation. In contrast, the most sensitive parameter in the partition equation (f_{oc}) only affects the SSL by a factor of 1.5.

Partition Equation. The partition equation requires the following site-specific inputs: fraction organic carbon, average annual soil moisture content, and soil bulk density. Although volumetric soil moisture content is somewhat dependent on bulk density (in terms of the porosity available to be filled with water), calculations were conducted to ensure that the parameter ranges selected do not result in impossible combinations of these parameters. Because the effects of the soil parameters on the SSLs are highly dependent on chemical properties, the analysis was conducted on four organic chemicals spanning the range of these properties: chloroform, trichloroethylene, naphthalene, and benzo(*a*)pyrene.

The range used for soil moisture conditions was 0.02 to 0.43 L water/L soil. The lower end of this range represents a likely residual moisture content value for sand, as might be found in the drier regions of the United States. The higher value (0.43) represents full saturation conditions for a loam soil. The range of bulk density (1.25 to 1.75) was obtained from the Patriot soils database, which contains bulk density measurements for over 20,000 soil series across the United States.

Establishing a range for subsurface organic carbon content (f_{oc}) was more difficult. In spite of an extensive literature review and contacts with soil scientists, very little information was found on the distribution of this parameter with depth in U.S. soils. The range used was 0.001 to 0.003 g carbon / g soil. The lower limit represents the critical organic carbon content below which the partition equation is no longer applicable. The upper limit was obtained from EPA's Environmental Research Laboratory in Ada, Oklahoma, as an expert opinion. Generally, soil organic carbon content falls off rapidly with depth. Since the typical value used as an SSL default for surface soils is 0.006, and 0.002 is used for subsurface soils, this limited range is consistent with the other default assumptions used in the Soil Screening Guidance.

The results of the partition equation sensitivity analysis are shown in Table 8.

For volatile chemicals, the model is somewhat sensitive to water content, with up to 54 and 19 percent change in SSLs for chloroform and trichloroethylene, respectively. The model is less sensitive to bulk density, with a high percent change of 18 for chloroform and 14 for trichloroethylene. Organic carbon content has the greatest effect on SSLs for all chemicals except chloroform. As expected, the effect of f_{oc} increases with increasing K_{oc}. The greatest effect was seen for benzo(*a*)pyrene whose SSL showed a 50 percent increase at an f_{oc} of 0.03. An f_{oc} of 0.005 will increase the benzo(*a*)pyrene SSL by 150 percent.

Table 8. Sensitivity Analysis for SSL Partition Equation

	Chloroform		Trichloroethylene		Naphthalene		Benzo(*a*)pyrene	
Parameter assignments	**SSL (mg/kg)**	**Percent change**	**SSL (mg/kg)**	**Percent change**	**SSL (mg/kg)**	**Percent change**	**SSL (mg/kg)**	**Percent change**
All default parameter values	0.59	—	0.057	—	84	—	8	—
Less conservative parameter value								
Organic carbon	0.67	14	0.074	29	124	48	12	50
Bulk density	0.69	18	0.065	14	85	1	8	0
Soil moisture	0.74	26	0.062	9	86	2	8	0
More conservative parameter value								
Organic carbon	0.51	-14	0.040	-29	44	-48	4	-50
Bulk density	0.51	-13	0.051	-10	83	-1	8	0
Soil moisture	0.27	-54	0.046	-19	80	-4	8	0

	Conservatism		
Input parameters	**Less**	**Nominal**	**More**
Fraction org. carbon (g/g)	0.003	0.002	0.001
Bulk density (kg/L)	1.25[a]	1.50	1.75[b]
Average soil moisture (L/L)	0.43	0.30	0.02

[a] n = 0.53; q_a = 0.23.

[b] n = 0.34; q_a = 0.04.

Chemical-specific parameters	**Chloroform**	**Trichloroethylene**	**Naphthalene**	**Benzo(*a*)pyrene**
K_{oc}	3.98E+01	1.66E+02	2.00E+03	1.02E+06
H'	1.50E-01	4.22E-01	1.98E-02	4.63E-05
C_w	2.0[c]	0.1[c]	20[d]	0.004[c]

[c] MCL × 20 DAF.

[d] HBL (HQ=1) × 20 DAF.

Dilution Factor. Site-specific parameters for the dilution factor model include aquifer hydraulic conductivity (K), hydraulic gradient (i), infiltration rate (I), aquifer thickness (d), and source length parallel to ground water flow (L). Because they are somewhat dependent, hydraulic conductivity and hydraulic gradient were treated together as Darcy velocity (K × i). The parameter ranges used for the dilution factor analysis represent the 10th and 90th percentile values taken from the HGDB and DNAPL site databases, with the geometric mean serving as the nominal value, as shown in Table 9.

Source length was varied by assuming square sources of 0.5 to 30 acres in size. Bounding estimates were conducted for each of these source sizes.
The results in Table 9 show that Darcy velocity has the greatest effect on the dilution factor, with a range of dilution factors from 1.2 to 85 for a 30-acre source and 2.1 to 263 for a 0.5-acre source. Infiltration rate has the next highest effect, followed by source size and aquifer thickness. Note that aquifer thickness has a profound effect on the influence of source size on the dilution factor. Thick aquifers show no source size effect because the increase in infiltration flux from a larger source is balanced by the increase in mixing zone depth, which increases dilution in the aquifer. For very thin aquifers, the mixing zone depth is limited by the aquifer thickness and the increased infiltration flux predominates, decreasing the dilution factor for larger sources.

2.6 Mass-Limit Model Development

This section describes the development of models to solve the mass-balance violations inherent in the infinite source models used to calculate SSLs for the inhalation and migration to ground water exposure pathways. The models developed are not finite source models per se, but are designed for use with the current infinite source models to provide a lower, mass-based limit for SSLs for the migration to ground water and inhalation exposure pathways for volatile and leachable contaminants. For each pathway, the mass-limit model calculates a soil concentration that corresponds to the release of all contaminants present within the source, at a constant health-based concentration, over the duration of exposure. These mass-based concentration limits are used as a minimum concentration for each SSL; below this concentration, a receptor point concentration time-averaged over the exposure period cannot exceed the health-based concentration on which it is based.

2.6.1 Mass Balance Issues. Infinite source models are subject to mass balance violations under certain conditions. Depending on a compound's volatility and solubility and the size of the source, modeled volatilization or leaching rates can result in a source being depleted in a shorter time than the exposure duration (or the flux over a 30- or 70-year duration would release a greater mass of contaminants than are present). Several commenters to the December 1994 draft Soil Screening Guidance expressed concern that it is unrealistic for total emissions over the duration of exposure to exceed the total mass of contaminants in a source. Using the soil saturation concentration (C_{sat}) and a 5- to 10-meter contaminant depth, one commentor calculated that mass balance would be violated by the SSL volatilization model for 25 percent of the SSL chemicals.

Short of finite source modeling, the limitations of which in soil screening are discussed in the draft *Technical Background Document for Soil Screening Guidance* (U.S. EPA, 1994i), there were two options identified for addressing mass-balance violations within the soil screening process:

- Shorten the exposure duration to a value that would reflect mass limitations given the volatilization rate calculated using the current method

Table 9. Sensitivity Analysis for SSL Dilution Factor Model

Parameter assignments	Dilution Factor			Mixing depth (m)	
	Source area				
	30-acre	0.5-acre	Ratio of 0.5-acre/30-acre	30-acre	0.5 acre
All central parameters	5.2	15	2.9	12	5.1
Less conservative					
Darcy velocity	85	263	3.1	12	4.8
Aquifer thickness	15	15	1.0	40	5.1
Infiltration rate	39	118	3.0	12	4.8
More conservative					
Darcy velocity	1.2	2.1	1.8	12	12
Aquifer thickness	2.1	9.1	4.3	3.0	3.0
Infiltration rate	3.2	8.7	2.7	12	5.5

Input parameters	Conservatism		
	Less	Nominal	More
Darcy velocity (DV, m/yr)	442	22	0.8
Aquifer thickness (da, m)	46	12	3
Infiltration rate (m/yr)	0.02	0.18	0.35

Parameter sources

Percentile	DV[a] (m/yr)	da[b] (m)
10th	0.8	3.0
25th	4	5.5
50th	22	11
75th	121	23
90th	442	46
Average:	800	28
Geomean:	22	12

[a] 300 DNAPL & HGDB sites.

[b] 208 HGDB sites.

- Change the volatilization rate to a value corresponding to the uniform release of the total mass of contaminants over the period of exposure.

The latter approach was taken in the draft Risk-Based Corrective Action (RBCA) screening methodology developed by the American Society for Testing and Materials (ASTM) (ASTM, 1994). As stated on page B6 of the RBCA guidance (B.6.6.6):

> In the event that the time-averaged flux exceeds that which would occur if all chemicals initially present in the surficial soil zone volatilized during the exposure period, then the volatilization factor is determined from a mass balance assuming that all chemical initially present in the surficial soil zone volatilizes during the exposure period.

This was selected over the exposure duration option because it is reasonably conservative for screening purposes (obviously, more contaminant cannot possibly volatilize from the soil) and it avoided the uncertainties associated with applying the current models to estimate source depletion rates.

In summary, the mass-limit approach offers the following advantages:

- It corrects the possible mass-balance violation in the infinite-source SSLs.
- It does not require development of a finite source model to calculate SSLs.
- It is appropriate for screening, being based on the conservative assumption that all of the contaminant present leaches or volatilizes over the period of exposure.
- It is easy to develop and implement, requiring only very simple algebraic equations and input parameters that are, with the exception of source depth, already used to calculate SSLs.

The derivation of these models is described below. It should be noted that the American Industrial Health Council (AIHC) independently developed identical models to solve the mass-balance violation as part of their public comments on the Soil Screening Guidance.

2.6.2 Migration to Ground Water Mass-Limit Model. For the migration to ground water pathway, the mass of contaminant leached from a contaminant source over a fixed exposure duration (ED) period can be calculated as

$$M_l = C_w \times I \times A_s \times ED \qquad \textbf{(47)}$$

where

M_l = mass of contaminant leached (g)
C_w = leachate contaminant concentration (mg/L or g/m^3)
I = infiltration rate (m/yr)
A_s = source area (m^2)
ED = exposure duration (yr).

The total mass of contaminants present in a source can be expressed as

$$M_T = C_t \times \rho_b \times A_s \times d_s \qquad \textbf{(48)}$$

where

M_T = total mass of contaminant present (g)
C_t = total soil contaminant concentration (mg/kg or g/Mg, dry basis)
ρ_b = dry soil bulk density (kg/L or Mg/m^3)
A_s = source area (m^2)
d_s = source depth (m).

To avoid a mass balance violation, the mass of contaminant leached cannot exceed the total mass of contaminants present (i.e., M_l cannot exceed M_T). Therefore, the maximum possible contaminant mass that can be leached from a source (assuming no volatilization or degradation) is M_T and the upper limit for M_l is

$$M_l = M_T$$

or

$$C_w \times I \times A_s \times ED = C_t \times \rho_b \times A_s \times d_s$$

Rearranging to solve for the total soil concentration (C_t) corresponding to this situation (i.e., maximum possible leaching)

Mass-Limit Model for Migration to Ground Water Pathway

$$C_t = (C_w \times I \times ED)/(\rho_b \times d_s) \qquad \textbf{(49)}$$

Parameter/Definition (units)	Default
C_t/screening level in soil (mg/kg)	–
C_w/target soil leachate concentration (mg/L)	(nonzero MCLG, MCL, or HBL) × 20 DAF
I/infiltration rate (m/yr)	site-specific
ED/exposure duration (yr)	70
ρ_b/dry soil bulk density (kg/L)	1.5
d_s/average source depth (m)	site-specific

This soil concentration (C_t) represents a lower limit for soil screening levels calculated for the migration to ground water pathway. It represents the soil concentration corresponding to complete release of soil contaminants over the ED time period at a constant soil leachate concentration (C_w). Below this C_t, the soil leachate concentration averaged over the ED time period cannot exceed C_w.

2.6.3 Inhalation Mass-Limit Model. The volatilization factor (VF) is basically the ratio of the total soil contaminant concentration to the air contaminant concentration. VF can be calculated as

$$VF = (Q/C) \times (C_T^o/J_s^{ave}) \times 10^{-10}\ m^2kg/cm^2mg \qquad \textbf{(50)}$$

where

VF = volatilization factor (m^3/kg)
Q/C = inverse concentration factor for air dispersion (g/m^2-s per kg/m^3)
C_T^o = total soil contaminant concentration at t=0 (mg/kg or g/Mg, dry basis)
J_s^{ave} = average rate of contaminant flux from the soil to the air (g/cm^2-s).

The total amount of contaminant contained within a finite source can be written as

$$M_t = C_T^o \times \rho_b \times A_s \times d_s \qquad \textbf{(51)}$$

where

M_t = total mass of contaminant within the source (g)
C_T^o = total soil contaminant concentration at t=0 (mg/kg or g/Mg, dry basis)
ρ_b = soil dry bulk density (kg/L = Mg/m^3)
A_s = area of source (m^2)
d_s = depth of source (m).

If all of the contaminant contained within a finite source is volatilized over a given averaging time period, the average volatilization flux can be calculated as

$$J_s^{ave} = M_t/[(A_s \times 10^4\ cm^2/m^2) \times (T \times 3.15E7\ s/yr)] \qquad \textbf{(52)}$$

where

T = exposure period (yr).

Substituting Equation 51 for M_t in Equation 52 yields

$$J_s^{ave} = (C_T^o \times \rho_b \times d_s) / (10^4\ cm^2/m^2 \times T \times 3.15E7\ s/yr) \qquad \textbf{(53)}$$

Rearranging Equation 53 yields

$$C_T^o/J_s^{ave} = (10^4\ \mathrm{cm^2/m^2} \times T \times 3.15E7\ \mathrm{s/yr})/(\rho_b \times d_s) \qquad \textbf{(54)}$$

Substituting Equation 54 into Equation 50 yields

Mass-Limit Model for Inhalation of Volatiles

$$VF = (Q/C) \times [(T \times 3.15E7\ \mathrm{s/yr})/(\rho_b \times d_s \times 10^6\ \mathrm{g/Mg})] \qquad \textbf{(55)}$$

Parameter/Definition (units)	Default
VF/volatilization factor (m^3/kg)	–
Q/C/inverse of mean conc. at center of source (g/m^2-s per kg/m^3)	Table 3
T/exposure interval (yr)	30
ρ_b/dry soil bulk density (kg/L)	1.5
d_s/average source depth (m)	site-specific

If the VF calculated using an infinite source volatilization model for a given contaminant is less than the VF calculated using Equation 55, then the assumption of an infinite source may be too conservative for that specific contaminant at that source. Consequently, VF, as calculated in Equation 55, could be considered a minimum value for VF.

2.7 Plant Uptake

Commentors have raised concerns that the ingestion of contaminated produce from homegrown gardens may be a significant exposure pathway. EPA evaluated empirical data on plant uptake, particularly the data presented in the *Technical Support Document for Land Application of Sewage Sludge*, often referred to as the "Sludge Rule" (U.S. EPA, 1992d).

EPA found that empirical plant uptake-response slopes were available for selected metals but that available data were insufficient to estimate plant uptake of organics. In an effort to obtain additional empirical data, EPA has jointly funded research with the State of California on plant uptake of organic contaminants. These studies support ongoing revisions to the indirect, multimedia exposure model CalTOX.

The Sludge Rule identified six metals of concern with empirical plant uptake data: arsenic, cadmium, mercury, nickel, selenium, and zinc. Plant uptake-response slopes were given for seven plant categories such as grains and cereals, leafy vegetables, root vegetables, and garden fruits. EPA evaluated the study conditions (e.g., soil pH, application matrix) and methods (e.g., geometric mean, default values) used to calculate the plant uptake-response slopes for each plant category and determined that the geometric mean slopes were generally appropriate for calculating SSLs for the soil-plant-human exposure pathway.

However, the geometric mean of empirical uptake-response slopes from the Sludge Rule must be interpreted with caution for several reasons. First, the dynamics of sludge-bound metals may differ from the dynamics of metals at contaminated sites. For example, the empirical data were derived from a variety of studies at different soil conditions using different forms of the metal (i.e., salt vs. nonsalt). In studies where the application matrix was sludge, the adsorption power of sludge in the presence of calcium ions may have reduced the amount of metal that is bioavailable to plants and, therefore, plant uptake may be greater in non-sludge-amended soils.

In addition to these confounding conditions, default values of 0.001 were assigned for plant uptake in studies where the measured value was below 0.001. A default value was needed to calculate the geometric mean uptake-response slope values. Moreover, considerable study-to-study variability is shown in the plant uptake-response slope values (up to 3 orders of magnitude for certain plant/metal combinations). This variability could result from varying soil characteristics or experimental conditions, but models have not been developed to relate changes in plant uptake to such conditions. Thus, the geometric mean values represent "typical" values from the experiments; actual values at specific sites could show marked variation depending on soil composition, chemistry, and/or plant type.

OERR has used the information in the Sludge Rule to identify six metals (arsenic, cadmium, mercury, nickel, selenium, and zinc) of potential concern through the soil-plant-human exposure pathway for consideration on a site-specific basis. The fact that these metals have been identified should not be misinterpreted to mean that other contaminants are not of potential concern for this pathway. Other EPA offices are looking at empirical data and models for estimating plant uptake of organic contaminants from soils and OERR will incorporate plant uptake of organics once these efforts are reviewed and finalized.

Methods for evaluating the soil-plant-human pathway are presented in Appendix G. Generic screening levels are calculated based on the uptake factors (i.e., bioconcentration factors [Br]) presented in the Sludge Rule. Generic plant SSLs are compared with generic SSLs based on direct ingestion as well as levels of inorganics in soil that have been reported to cause phytotoxicity (Will and Suter, 1994). Although site-specific factors such as soil type, pH, plant type, and chemical form will determine the significance of this pathway, the results of our analysis suggest that the soil-plant-human pathway may be of particular concern for sites with soils contaminated with arsenic or cadmium. Likewise, the potential for phytotoxicity will be greatly influenced by site-specific factors; however, the data presented by Will and Suter (1994) suggest that, with the exception of arsenic, the levels of inorganics that are considered toxic to plants are well below the levels that may impact human health via the soil-plant-human pathway.

2.8 Intrusion of Volatiles into Basements: Johnson and Ettinger Model

Concern about the potential impact of contaminated soil on indoor air quality prompted EPA to consider the Johnson and Ettinger (1991) model, a heuristic model for estimating the intrusion rate of contaminant vapors from soil into buildings. The model is a closed-form analytical solution for both convective and diffusive transport of vapor-phase contaminants into enclosed structures located above the contaminated soil. The model may be solved for both steady-state (i.e., infinite source) or quasi-steady-state (i.e., finite source) conditions. The model incorporates a number of key assumptions, including no leaching of contaminant to ground water, no sinks in the building, and well-mixed air volume within the building.

To evaluate the effects of using the Johnson and Ettinger model on SSLs for volatile organic contaminants, EPA contracted Environmental Quality Management, Inc. (EQ), to construct a case example to estimate a high-end exposure point concentration for residential land use (Appendix H; EQ and Pechan, 1994). The case example models a contaminant source relatively close or directly beneath a building where the soil beneath the building is very permeable and the building is underpressurized, tending to pull contaminants into the basement. Where possible and appropriate, values of model variables were taken directly from Johnson and Ettinger (1991). Using both steady-state and quasi-steady-state formulations, building air concentrations of each of 42 volatile SSL chemicals were calculated. The inverses of these concentrations were substituted into the inhalation SSL equations (Equations 4 or 5) as an indoor volatilization factor (VF_{indoor}) to calculate carcinogenic or noncarcinogenic SSLs based on migration of contaminants into basements (i.e., "indoor inhalation" SSLs).

Results showed a difference of up to 2 orders of magnitude between the steady-state and quasi-steady-state results for the indoor inhalation SSLs. Infinite source indoor inhalation SSLs were less than the corresponding "outdoor" inhalation SSLs by as much as 3 orders of magnitude for highly volatile constituents. For low-volatility constituents, the difference was considerably less, with no difference in the indoor and outdoor SSLs in some cases. The EQ study also indicated that the most important input parameters affecting long-term building concentration (and thus the SSL) are building ventilation rate, distance from the source (i.e., source-building separation), soil permeability to vapor flow, and source depth. For lower-permeability soils, the number and size of cracks in the basement walls may be more significant, although this was not a significant variable for the permeable soils considered in the study.

EPA decided against using the Johnson and Ettinger model to calculate **generic** SSLs due to the sensitivity of the model to parameters that do not lend themselves to standardization on a national basis (e.g., source depth, the number and size of cracks in basement walls). In addition, the only formal validation study identified by EPA compares model results with measured radon concentrations from a highly permeable soil. Although these results compare favorably, it is not clear how applicable they are to less permeable soils and compounds not already present in soil as a gas (as radon is).

The model can be applied on a site-specific basis in conjunction with the results of a soil gas survey. Where land use is currently residential, a soil gas survey can be used to measure the vapor phase concentrations at the foundation of buildings, thereby eliminating the need to model partitioning of contaminants, migration from the source to the basement, and soil permeability.

For future use scenarios, although some site-specific data are available, the difficulties are similar to those encountered with generic application of the model. Predictions must be made regarding the distance from the source to the basement and the permeability of the soil, basement floor, and walls. EQ's report models the potential impact of placing a structure directly above the source. Depending on the permeability of the surrounding soils, the results suggest that the level of residual contamination would have to be extremely low to allow for such a scenario. Distance from the source can have a dramatic impact on the results and should be considered in more detailed investigations involving future residential use scenarios.