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Risk Assessment Technical Background Document for the Chlorinated Aliphatics Listing Determination

Appendixes

Prepared by
Center for Environmental Analysis
Research Triangle Institute
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U.S. Environmental Protection Agency
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July 30, 1999

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Appendices A - K

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Appendix A

Glossary of Terms

Appendix A

GLOSSARY OF TERMS

Ambient - The conditions surrounding a person, sampling location, etc.

Arithmetic mean - The sum of all the measurements in a data set divided by the number of measurements in the data set.

Blank (blank sample) - An unexposed sampling medium, or an aliquot of the reagents used in an analytical procedure, in the absence of added analyte. The measured value of a blank sample is the blank value.

Dose - The amount of a substance available for interaction with metabolic processes or biologically significant receptors after crossing the outer boundary of an organism. The potential dose is the amount ingested, inhaled, or applied to the skin. The applied dose is the amount of a substance presented to an absorption barrier and available for absorption (although not necessarily having yet crossed the outer boundary of the organism). The absorbed dose is the amount crossing a specific absorption barrier (e.g., the exchange boundaries of skin, lung, and digestive tract) through uptake processes. Internal dose is a more general term denoting the amount absorbed without respect to specific absorption barriers or exchange boundaries. The amount of the chemical available for interaction by any particular organ or cell is termed the delivered dose for that organ or cell.

Dose-response assessment - The determination of the relationship between the magnitude of administered, applied, or internal dose and a specific biological response. Response can be expressed as measured or observed incidence, percent response in groups of subjects (or populations), or the probability of occurrence of a response in a population.

Dose-response curve - A graphical representation of the quantitative relationship between administered, applied, or internal dose of a chemical or agent, and a specific biological response to that chemical or agent.

Dose-response relationship - The resulting biological responses in an organ or organism expressed as a function of a series of different doses.

Environmental fate - The destiny of a chemical or biological pollutant after release into the environment. Environmental fate involves temporal and spatial considerations of transport, transfer, storage, and transformation.

Environmental fate model - In the context of exposure assessment, any mathematical abstraction of a physical system used to predict the concentration of specific chemicals as a function of space and time subject to transport, intermedia transfer, storage, and degradation in the environment.

Environmental medium - One of the major categories of material found in the physical environment that surrounds or contacts organisms, e.g., surface water, ground water, soil, or air, and through which chemicals or pollutants can move and reach the organisms.

Exposure - Contact of a chemical, physical, or biological agent with the outer boundary of an organism. Exposure is quantified as the concentration of the agent in the medium in contact integrated over the time duration of that contact.

Exposure assessment - The determination or estimation (qualitative or quantitative) of the magnitude, frequency, duration, and route of exposure.

Exposure point concentration - The concentration of a chemical in its transport or carrier medium at the point of contact.

Exposure pathway - The physical course a chemical or pollutant takes from the source to the organism exposed.

Exposure route - The way a chemical or pollutant enters an organism after contact, e.g., by ingestion, inhalation, or dermal absorption.

Exposure scenario - A set of facts, assumptions, and inferences about how exposure takes place that aids the exposure assessor in evaluating, estimating, or quantifying exposures.

Hazard identification - A description of the potential health effects attributable to a specific chemical or physical agent. For carcinogen assessments, the hazard identification phase of a risk assessment is also used to determine whether a particular agent or chemical is, or is not, causally linked to cancer in humans.

High-end exposure (dose) estimate - A plausible estimate of individual exposure or dose for those persons at the upper end of an exposure or dose distribution, conceptually above the 90th percentile, but not higher than the individual in the population who has the highest exposure or dose.

High-end Risk Descriptor - A plausible estimate of the individual risk for those persons at the upper end of the risk distribution, conceptually above the 90th percentile but not higher than the individual in the population with the highest risk. Note that persons in the high end of the risk distribution have high risk due to high exposure, high susceptibility, or other reasons, and therefore persons in the high end of the exposure or dose distribution are not necessarily the same individuals as those in the high end of the risk distribution.

Intake - The process by which a substance crosses the outer boundary of an organism without passing an absorption barrier, e.g., through ingestion or inhalation.

Median value - The value in a measurement data set such that half the measured values are greater and half are less.

Monte Carlo technique - A repeated random sampling from the distribution of values for each of the parameters in a generic (exposure or dose) equation to derive an estimate of the distribution of (exposures or doses in) the population.

Pathway - The physical course a chemical or pollutant takes from the source to the organism exposed.

Quality assurance (QA) - An integrated system of activities involving planning, quality control, quality assessment, reporting and quality improvement to ensure that a product or service meets defined standards of quality with a stated level of confidence.

Quality control (QC) - The overall system of technical activities whose purpose is to measure and control the quality of a product or service so that it meets the needs of the users. The aim is to provide quality that is satisfactory, adequate, dependable, and economical.

Range - The difference between the largest and smallest values in a measurement data set.

Representativeness - The degree to which a sample is, or samples are, characteristic of the whole medium, exposure, or dose for which the samples are being used to make inferences.

Risk - The probability of deleterious health or environmental effects.

Risk characterization - The description of the nature and often the magnitude of human or nonhuman risk, including attendant uncertainty.

Risk descriptors - Statements to convey information about risk to users of that information, primarily risk managers. Risk descriptors can be grouped as descriptors of individual risk or population risk, and within these broad categories, there are several types of descriptors.

Route - The way a chemical or pollutant enters an organism after contact, e.g., by ingestion, inhalation, or dermal absorption.

Sample - A small part of something designed to show the nature or quality of the whole. Exposure-related measurements are usually samples of environmental or ambient media, exposures of a small subset of a population for a short time, or biological samples, all for the purpose of inferring the nature and quality of parameters important to evaluating exposure.

Sampling plan - A set of rules or procedures specifying how a sample is to be selected and handled.

Scenario evaluation - An approach to quantifying exposure by measurement or estimation of both the amount of a substance contacted, and the frequency/duration of contact, and subsequently linking these together to estimate exposure or dose.

Uptake - The process by which a substance crosses an absorption barrier and is absorbed into the body.

Appendix B

Groundwater Pathway Screening Analyses

Table B-1 Groundwater Pathway Screening Analysis for EDC/VCM Sludge Managed in a Land Treatment Unit.

Constituent	CAS	Predicted Leachate Concentration (ug/L)	Drinking Water Ingestion Rate (L/day)	Exposure Duration (yr)	Exposure Frequency (days/yr)	Body Weight (kg)	Average Daily Intake (mg/kg/day)	Oral CSF (mg/kg/day)-1	RfD (mg/kg/day)	Cancer Risk	Hazard Quotient
Dry Weight Waste Concentrations											
VOCs & Semi-VOCs											
Benzoic acid	65-85-0	1.39E-01	0.74	9	350	21.4	4.6E-06	NA	4.0E+00	NAP	0.000001
Acetone	67-64-1	1.12E+00	0.74	9	350	21.4	3.7E-05	NA	1.0E-01	NAP	0.0004
Chloroform	67-66-3	3.03E-02	1.4	58.4	350	70	4.8E-07	6.1E-03	1.0E-02	3E-09	a
Vinyl chloride	75-01-4	3.35E-03	1.4	58.4	350	70	5.4E-08	1.9E+00	NA	1E-07	NAP
Methylene chloride	75-09-2	8.72E-03	1.4	58.4	350	70	1.4E-07	7.5E-03	6.0E-02	1E-09	a
Carbon disulfide	75-15-0	2.00E-03	0.74	9	350	21.4	6.6E-08	NA	1.0E-01	NAP	0.0000007
Methyl ethyl ketone	78-93-3	4.84E-02	0.74	9	350	21.4	1.6E-06	NA	6.0E-01	NAP	0.000003
Trichloroethylene	79-01-6	1.61E-05	1.4	58.4	350	70	2.6E-10	1.1E-02	NA	3E-12	NAP
Allyl chloride	107-05-1	5.17E-04	1.4	58.4	350	70	8.3E-09	2.1E-02	NA	2E-10	NAP
Dichloroethane, 1,2-	107-06-2	8.12E-02	1.4	58.4	350	70	1.3E-06	9.1E-02	NA	1E-07	NAP
Vinyl acetate	108-05-4	2.82E-03	0.74	9	350	21.4	9.3E-08	NA	1.0E+00	NAP	0.0000001
Bis(2-chlorethyl)ether	111-44-4	5.72E-01	1.4	58.4	350	70	9.1E-06	1.1E+00	NA	**1E-05**	NAP
Bis(2-ethylhexyl)phthalate	117-81-7	1.02E-05	1.4	58.4	350	70	1.6E-10	1.4E-02	2.0E-02	2E-12	a
Hexachlorobenzene	118-74-1	4.35E-05	1.4	58.4	350	70	7.0E-10	1.6E+00	8.0E-04	1E-09	a
Tetrachloroethylene	127-18-4	2.08E-04	1.4	58.4	350	70	3.3E-09	5.2E-02	1.0E-02	2E-10	a
Metals											
Aluminum	7429-90-5	1.04E+04	0.74	9	350	21.4	3.5E-01	NA	NA	NAP	NAP
Lead	7439-92-1	5.03E+00	0.74	9	350	21.4	1.7E-04	NA	NA	NAP	NAP
Manganese	7439-96-5	1.72E+03	0.74	9	350	21.4	5.7E-02	NA	1.4E-01	NAP	0.4
Molybdenum	7439-98-7	1.32E+01	0.74	9	350	21.4	4.4E-04	NA	5.0E-03	NAP	0.09
Nickel	7440-02-0	2.91E+02	0.74	9	350	21.4	9.6E-03	NA	2.0E-02	NAP	0.5
Arsenic	7440-38-2	5.22E+01	1.4	58.4	350	70	8.4E-04	1.5E+00	3.0E-04	**1E-03**	a
Barium	7440-39-3	2.89E+02	0.74	9	350	21.4	9.6E-03	NA	7.0E-02	NAP	0.1
Cadmium	7440-43-9	2.06E+00	0.74	9	350	21.4	6.8E-05	NA	5.0E-04	NAP	0.1
Chromium	7440-47-3	1.72E+02	0.74	9	350	21.4	5.7E-03	NA	3.0E-03	NAP	**2**
Cobalt	7440-48-4	3.02E+01	0.74	9	350	21.4	1.0E-03	NA	6.0E-02	NAP	0.02
Copper	7440-50-8	1.84E+04	0.74	9	350	21.4	6.1E-01	NA	NA	NAP	NAP
Vanadium	7440-62-2	3.26E+00	0.74	9	350	21.4	1.1E-04	NA	7.0E-03	NAP	0.02
Zinc	7440-66-6	2.05E+03	0.74	9	350	21.4	6.8E-02	NA	3.0E-01	NAP	0.2

Table B-1 Groundwater Pathway Screening Analysis for EDC/VCM Sludge Managed in a Land Treatment Unit.

Constituent	CAS	Predicted Leachate Concentration (ug/L)	Drinking Water Ingestion Rate (L/day)	Exposure Duration (yr)	Exposure Frequency (days/yr)	Body Weight (kg)	Average Daily Intake (mg/kg/day)	Oral CSF (mg/kg/day)-1	RfD (mg/kg/day)	Cancer Risk	Hazard Quotient
Dioxins and Furans											
2,3,7,8-TCDD	1746-01-6	1.01E-07	1.4	58.4	350	70	1.6E-12	1.6E+05	NA	3E-07	NAP
1,2,3,4,5,7,8,9-OCDD	3268-87-9	2.74E-06	1.4	58.4	350	70	4.4E-11	1.6E+02	NA	7E-09	NAP
1,2,3,7,8,9-HxCDD	19408-74-3	4.48E-08	1.4	58.4	350	70	7.2E-13	1.6E+04	NA	1E-08	NAP
1,2,3,4,6,7,8-HpCDD	35822-46-9	7.74E-08	1.4	58.4	350	70	1.2E-12	1.6E+03	NA	2E-09	NAP
OCDF	39001-02-0	5.50E-06	1.4	58.4	350	70	8.8E-11	1.6E+02	NA	1E-08	NAP
1,2,3,4,7,8-HxCDD	39227-28-6	8.87E-10	1.4	58.4	350	70	1.4E-14	1.6E+04	NA	2E-10	NAP
2,3,7,8-TCDF	51207-31-9	5.07E-07	1.4	58.4	350	70	8.1E-12	1.6E+04	NA	1E-07	NAP
1,2,3,4,7,8,9-HpCDF	55673-89-7	2.37E-06	1.4	58.4	350	70	3.8E-11	1.6E+03	NA	6E-08	NAP
2,3,4,7,8-PeCDF	57117-31-4	2.10E-07	1.4	58.4	350	70	3.4E-12	7.8E+04	NA	3E-07	NAP
1,2,3,7,8-PeCDF	57117-41-6	7.82E-09	1.4	58.4	350	70	1.3E-13	7.8E+03	NA	1E-09	NAP
1,2,3,6,7,8-HxCDF	57117-44-9	2.73E-08	1.4	58.4	350	70	4.4E-13	1.6E+04	NA	7E-09	NAP
1,2,3,6,7,8-HxCDD	57653-85-7	5.97E-08	1.4	58.4	350	70	9.6E-13	1.6E+04	NA	1E-08	NAP
2,3,4,6,7,8-HxCDF	60851-34-5	4.72E-07	1.4	58.4	350	70	7.6E-12	1.6E+04	NA	1E-07	NAP
1,2,3,4,6,7,8-HpCDF	67562-39-4	3.64E-06	1.4	58.4	350	70	5.8E-11	1.6E+03	NA	9E-08	NAP
1,2,3,4,7,8-HxCDF	70648-26-9	1.01E-06	1.4	58.4	350	70	1.6E-11	1.6E+04	NA	3E-07	NAP
1,2,3,7,8,9-HxCDF	72918-21-9	1.23E-08	1.4	58.4	350	70	2.0E-13	1.6E+04	NA	3E-09	NAP
Wet Weight Waste Concentration, Infiltration = 0.5893m/yr											
Bis(2-chlorethyl)ether	111-44-4	2.43E-01	1.4	58.4	350	70	3.9E-06	1.1E+00	NA	**4E-06**	NAP
Arsenic	7440-38-2	1.31E+01	1.4	58.4	350	70	2.1E-04	1.5E+00	3.0E-04	**3E-04**	a
Chromium	7440-47-3	4.40E+01	0.74	9	350	21.4	1.5E-03	NA	3.0E-03	NAP	0.5

CSF - Cancer slope factor.
RfD - Reference dose
HQ - Hazard quotient.
NA - Not available.
NAP - Not applicable.
a - Only cancer risk was calculated.

Table B-2 Groundwater Pathway Screening Analysis for EDC/VCM Sludge Managed in a Landfill

Constituent	CAS	TCLP Concentration (mg/L)	Drinking Water Ingestion Rate (L/day)	Exposure Duration (yr)	Exposure Frequency (days/yr)	Body Weight (kg)	Average Daily Intake (mg/kg/day)	Oral CSF (mg/kg/day)-1	RfD (mg/kg/day)	Cancer Risk	Hazard Quotient
VOCs & Semi-VOCs											
Benzoic acid	65-85-0	1.08E-01	0.74	9	350	21.4	0.0036	NA	4	NAP	0.0009
Acetone	67-64-1	6.70E-01	0.74	9	350	21.4	0.022	NA	0.1	NAP	0.2
Chloroform	67-66-3	3.20E-02	1.4	58.4	350	70	0.0005	0.0061	0.01	**3E-06**	a
Methylene chloride	75-09-2	4.40E-02	1.4	58.4	350	70	0.0007	0.0075	0.06	**5E-06**	a
Carbon disulfide	75-15-0	7.20E-03	0.74	9	350	21.4	0.0002	NA	0.1	NAP	0.002
Methyl ethyl ketone	78-93-3	2.80E-02	0.74	9	350	21.4	0.00093	NA	0.6	NAP	0.002
Methylphenol, 4-	106-44-5	4.20E-02	0.74	9	350	21.4	0.0015	NA	0.005	NAP	0.29
Dichloroethane, 1,2-	107-06-2	3.60E-02	1.4	58.4	350	70	0.0006	0.091	NA	**5E-05**	NAP
Methyl-2-pentanone, 4-	108-10-1	3.70E-03	0.74	9	350	21.4	0.0001	NA	0.08	NAP	0.002
Bis(2-chloroethyl)ether	111-44-4	1.20E-02	1.4	58.4	350	70	0.00019	1.1	NA	**2E-04**	NAP
Dichloropropene, cis-1,3-	10061-01-5	3.80E-03	1.4	58.4	350	70	0.00006	0.18	0.0003	**1E-05**	a
Metals											
Manganese	7439-96-5	1.29E+01	0.74	9	350	21.4	0.42774	NA	0.14	NAP	**3**
Molybdenum	7439-98-7	2.20E-01	0.74	9	350	21.4	0.007295	NA	0.005	NAP	**1**
Nickel	7440-02-0	1.30E+00	0.74	9	350	21.4	0.045	NA	0.02	NAP	**2**
Arsenic	7440-38-2	5.30E-02	1.40	58.4	350	70	0.0008	1.5	0.0003	**1E-03**	a
Cobalt	7440-48-4	7.00E-02	0.74	9	350	21.4	0.002321	NA	0.06	NAP	0.04
Copper	7440-50-8	2.23E+01	0.74	9	350	21.4	0.77	NA	NA	NAP	NAP
Zinc	7440-66-6	4.00E+00	0.74	9	350	21.4	0.13263	NA	0.3	NAP	0.4
Dioxins											
OCDD	3268-87-9	2.00E-07	1.4	58.4	350	70	0.000000003	156	NA	5E-07	NAP
OCDF	39001-02-0	9.90E-05	1.4	58.4	350	70	0.0000016	156	NA	**2E-04**	NAP
1,2,3,4,7,8,9-HpCDF	55673-89-7	4.00E-07	1.4	58.4	350	70	0.00000001	1560	NA	**1E-05**	NAP
1,2,3,4,6,7,8-HpCDF	67562-39-4	1.10E-06	1.4	58.4	350	70	0.00000002	1560	NA	**3E-05**	NAP

CSF - Cancer slope factor.
RfD - Reference dose
HQ - Hazard quotient.
NA - Not available.
NAP - Not applicable.
a - Only cancer risk was calculated.

Table B-3 Groundwater Pathway Screening Analysis for Methyl Chloride Sludge Managed in a Landfill

Constituent	CAS No.	TCLP Concentration (mg/L)	Drinking Water Ingestion Rate (L/day)	Expsosure Duration (yr)	Exposure Frequency (days/yr)	Body Weight (kg)	Average Daily Intake (mg/kg/day)	Oral CSF (mg/kg/day)-1	RfD (mg/kg/day)	Cancer Risk	HQ
Benzoic acid	65-85-0	0.01	0.74	9	350	21.4	0.0004	NA	4	NAP	0.0001
Acetone	67-64-1	0.2	0.74	9	350	21.4	0.005	NA	0.1	NAP	0.05
Methylene chloride	75-09-2	0.009	1.4	58.4	350	70	0.0001	7.5E-03	0.06	1E-06	a
Carbon disulfide	75-15-0	0.006	0.74	9	350	21.4	0.0002	NA	0.1	NAP	0.002
Manganese	7439-96-5	4	0.74	9	350	21.4	0.1	NA	0.14	NAP	1
Arsenic	7440-38-2	0.002	1.4	58.4	350	70	0.00003	1.5	0.0003	**5E-05**	a
Copper	7440-50-8	5	0.74	9	350	21.4	0.2	NA	NA	NAP	NAP
Zinc	7440-66-6	11	0.74	9	350	21.4	0.4	NA	0.3	NAP	1

CSF - Cancer slope factor.
RfD - Reference dose
HQ - Hazard quotient.
NA - Not available.
NAP - Not applicable.
a - Only cancer risk was calculated.

Appendix C

Chemical Specific Parameters

Table C-1. Chemical-Specific Inputs for Acetone

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	5.8E-1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	5.8E-1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	3.03E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1E+6	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	58.08	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	3.88E-5	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1.2E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	8E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	8.4E-1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.3E+1	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.4E-8	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	4.6E-9	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.7E-4	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	1.69E-1	U.S. EPA, 1991
Other Parameters			
Fw	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	3.6E+1	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	1E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-2. Chemical-Specific Inputs for Allyl chloride

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	2.7E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	2.8E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	4.84E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	3.37E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	76.53	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.1E-2	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1.2E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.8E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.2	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.6	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	7.1E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	2.2E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	7E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	3.66	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	18	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	2.1E-2	CalEPA, 1997
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	1E-3	U.S. EPA, 1998a (IRIS)

NA = Not Available.

[1] The value presented is not a biodegradation rate, but was based on hydrolysis rate and was estimated as ln2/soil half-life.

Table C-3. Chemical-Specific Inputs for Benzoic acid

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	6.7E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	7.2E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	6.79E-6	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	3.5E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	122.12	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.54E-6	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	5.4E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	3.5E+2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.6	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	3.3	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.8E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	5.8E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	7.2E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	6.1	Isnard et al., 1988
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	4	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-4. Chemical-Specific Inputs for Benzyl alcohol

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.2E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.3E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	8.2E-5	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	4.0E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	108.14	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	2.2E-7	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.1E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	9.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	3.8E+2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.0	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	8.8	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	3.2E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.0E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	2.6E-03	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	1.97	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	3.0E-1	U.S. EPA, 1997a (HEAST)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-5. Chemical-Specific Inputs for Bis(2-chlorethyl)ether

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.5E+1	Calculated[1] (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.6E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.0E-3	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.7E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	143.01	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.8E-5	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	6.9E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	7.5E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	6	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	7.7	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	4.1E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.3E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.8E-03	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	3.22	Veith et al., 1980
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	1.4	Howard et al., 1991[2]
K_n^{25}	Neutral Hydrolysis Rate Constant (y^{-1})	0.23	Kollig, 1993
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.1	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	3.3E-4	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] K_{oc} value for analysis of the groundwater pathway was 6.31 cm^3/g.

[2] The soil biodegradation rate was estimated as ln2/soil half-life.

2-(2-chloroethoxy)ethanol is a daughter product of Bis(2-chloroethyl)ether and was evaluated for the groundwater pathway only. The K_{oc} value for 2-(2-chloroethoxy)ethanol is 0.65 cm^3/g. The K_n^{25} value for 2-(2-chloroethoxy)ethanol is 0.28 y^{-1}.

1,4-Dioxane is a daughter product of Bis(2-chloroethyl)ether and was evaluated for the groundwater pathway only. The K_{oc} value for 1,4-Dioxane is 0.15 cm^3/g.

Table C-6. Chemical-Specific Inputs for Bis(2-ethylhexyl)phthalate

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.5E+7	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	2.0E+7	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	8.49E-9	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	3.4E-1	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	390.56	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.02E-7	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	3.5E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	3.7E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	8.2E+7	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.3E+4	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	5E-1	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.6E-1	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	1.19E+2	Stephan, 1993[1]
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	NA	
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	11	Howard et al., 1991[2]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.4E-2	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	2E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] For Bis(2-ethylhexyl)phthalate is a single measured BCF in Stephan (1993) and is used as a surrogate BAF because the predicted values are inappropriate for chemicals with log Kow > 6.5.

[2] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-7. Chemical-Specific Inputs for Bis(2-chloroisopropyl)ether

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	3.4E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	3.8E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.0E-3[1]	Verschueren, 1983
Sol	Water solubility (mg/L)	1.3E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	171.04	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.5E-4	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	6.0E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	6.4E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	21.0	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	3.7	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.2	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	9.5E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	3.0E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.2E-02	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	28.6	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	7.0E-2[2]	U.S. EPA, 1997a (HEAST)
RfD	Reference Dose (mg/kg/day)	4.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	1.0E-5[2]	U.S. EPA, 1997a (HEAST)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] In Verschueren (1983) the vapor pressure was calculated at 20 degrees Celsius instead of 25 degrees Celsius.

[2] The health benchmark numbers are for Bis(2-chloro-1-methyl ethyl)ether (CAS # 108-60-1). This compound contained 70% Bis(2-chloro-1-methyl ethyl)ether and 30% Bis(2-chloroisopropyl) ether.

Table C-8. Chemical-Specific Inputs for Bromodichloromethane

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.2E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.3E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	6.6E-2	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	6.7E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	163.83	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.6E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	3.0E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	6.0E-1	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	2.1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.4	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	3.2E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.0E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.9E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	11.9	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	6.2E-2	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	2.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-9. Chemical-Specific Inputs for Bromoform

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
Koc	Soil Adsorbtion Coefficient (mL/g)	2E+2	Calculated (Di Toro et al., 1991)
Kow	Octanol-water partition coefficient (unitless)	2.2E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	7.25E-3	U.S. EPA, 1996b (SCDM)
SOl	Water solubility (mg/L)	3.1E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	252.73	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	5.35E-4	Calculated
D_a	Diffusivity in air (cm^2/sec)	1.5E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	3.3	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	2.8	Calculated (U.S. EPA, 1993)
$BCF_{Plant\text{-}Soil}$	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.7	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	5.6E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.8E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	2.6E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	1.88E+1	U.S. EPA, 1991
Other Parameters			
Fw	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	1.4	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	7.9E-3	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	2E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	1.1E-6	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-10. Chemical-Specific Inputs for Carbon disulfide

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	9.3E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	4.72E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.19E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	76.14	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	3.02E-2	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2.5E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.9	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.7	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.5E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	7.9E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.7E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	9.95	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	1E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	7E-1	U.S. EPA, 1998a (IRIS)

NA = Not Available.

Table C-11. Chemical-Specific Inputs for 2-Chloro-1,3-butadiene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.1E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.2E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.8E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.7E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	88.54	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.4E-2	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1.0E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.0E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	6.4E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	2.0	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.4	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	3.0E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	9.5E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.6E-02	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	11.5	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	2.0E-2	U.S. EPA, 1997a (HEAST)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	7.0E-3	U.S. EPA, 1997a (HEAST)

NA = Not Available.

Table C-12. Chemical-Specific Inputs for Chlorobenzene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	6.5E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	7.2E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.6E-2	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	4.7E+2	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	112.56	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	3.7E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.3E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	8.7E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.7	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	5.6	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	.86	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.8E-5	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	5.8E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	4.2E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	87.4	Lyman et al., 1990
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	2.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	2.0E-2	U.S. EPA, 1997a (HEAST)

NA = Not Available.

Table C-13. Chemical-Specific Inputs for Chlorodibromomethane

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.4E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.5E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	6.5E-3	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.6E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	208.28	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	7.8E-4	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	2.0E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.5	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	2.2	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.2	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	3.7E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.2E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	3.5E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	13.6	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	1.4	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	8.4E-2	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	2.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-14. Chemical-Specific Inputs for Chloroform

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	7.7E+1	Calculated[1] (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	8.3E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.59E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	7.92E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	119.38	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	3.67E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.7E-1	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.7	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	3	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.1E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	6.6E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	8.2E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	2.62	MacKay, 1982
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	1.4	Howard et al., 1991[2]
K_n^{25}	Neutral Hydrolysis Rate Constant (y^{-1})	1E-4	Kollig, 1993
K_b^{25}	Base Second-order Rate Constant ($M^{-1}Y^{-1}$)	2.7E+3	Kollig, 1993
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	6.1E-3	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	1E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	2.3E-5	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] K_{oc} value for anaylsis of the groundwater pathway was 38.02 cm^3/g.

[2] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-15. Chemical-Specific Inputs for o-Cresol

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	9.0E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	9.8E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	3.9E-4	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.6E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	108.14	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.2E-6	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.4E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	8.3E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	6.1E+2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.8	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.7	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.5E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	7.8E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.1E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	9.77	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	5.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-16. Chemical-Specific Inputs for p-Cresol

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	8.3E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	8.9E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.4E-4	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.15E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	108.14	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	7.92E-7	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.4E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.0E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	8.4E+2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.8	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.9	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.2E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	7.1E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.0E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	9.08	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	5.0E-3	U.S. EPA, 1997a (HEAST)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-17. Chemical-Specific Inputs for 1,2 Dichloroethane

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	2.8E+1	Calculated[1] (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	3E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.04E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	8.52E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	98.96	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	9.79E-4	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	9.9E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2.1E-1	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.2	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.5	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	7.4E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	2.3E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.2E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	5.07	Veith et al., 1980
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	1.4	Howard et al., 1991[2]
K_n^{25}	Neutral Hydrolysis Rate Constant (y^{-1})	9.3E-3	Kollig, 1993
K_b^{25}	Base Second-order Rate Constant (M^{-1}Y^{-1})	54.7	Kollig, 1993
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	9.1E-2	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	2.6E-5	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] K_{oc} value for analysis of the groundwater pathway was 13.49 cm^3/g.

[2] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-18. Chemical-Specific Inputs for cis-1,2-Dichloroethylene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	6.7E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	7.2E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.7E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	3.5E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	96.94	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	4.1E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.3E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.1E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	0.13	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.6	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	3.3	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.8E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	5.8E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.0E-02	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	7.7	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	1.0E-2	U.S. EPA, 1997a (HEAST)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-19. Chemical-Specific Inputs for trans-1,2-Dichloroethylene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.1E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.2E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	4.4E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	6.3E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	96.94	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	9.4E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.0E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.2E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	9.5E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	2.0	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.5	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	3.0E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	9.3E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.4E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration Factor (L/kg)	11.3	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	2.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-20. Chemical-Specific Inputs for Diethyl phthalate

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	2.9E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	3.2E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.2E-6	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.1E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	222.24	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	4.5E-7	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	2.6E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	6.4E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g air])	5.7E+3	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([μg pollutant/g plant tissue FW]/[μg pollutant/mL soil water])	3.4	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g soil])	1.4	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	7.9E-6	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	2.5E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.0E-03	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	47.2	Lyman et al., 1990
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	8.0E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per μg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-21. Chemical-Specific Inputs for Dimethyl phthalate

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	3.5E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	3.7E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.2E-6	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	4.0E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	194.19	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.1E-7	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	5.7E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	6.3E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2.5E+3	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.3	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	4.8	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	9.3E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	3.0E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.6E-03	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	9.16	Lyman et al., 1990
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-22. Chemical-Specific Inputs for Di-n-octyl phthalate

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	8.4E+7	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.1E+8	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	3.4E-9	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.0E-2	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	390.56	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	6.7E-5	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1.5E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	3.6E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	8.0E+5	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	4.9E+4	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	8.5E-4	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.9	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	.91	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	4.2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	1.19E+2	Stephan, 1993[1]
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	NA	
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	2.0E-2	U.S. EPA, 1997a (HEAST)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] Stephan (1993) used a predicted HHBAF value for DEHP because there was a lack of information for Di-n-octyl phthalate and there was a similarity between the two chemicals.

Table C-23. Chemical-Specific Inputs for Ethylbenzene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.2E+3	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.4E+3	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.3E-2	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.7E+2	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	106.17	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	7.9E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.5E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	7.8E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.6	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	8.7	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	.59	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	3.5E-5	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.1E-5	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	7.3E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	79.1	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	1.0E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	1.0	U.S. EPA, 1998a (IRIS)

NA = Not Available.

Table C-24. Chemical-Specific Inputs for Ethyl chloride

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	2.5E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	2.7E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.3	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	5.7E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	64.51	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	8.8E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	2.7E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.2E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2.1E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.2	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.8	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	6.8E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	2.1E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	8.0E-03	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	3.54	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	1.0E+1	U.S. EPA, 1998a (IRIS)

NA = Not Available.

Table C-25. Chemical-Specific Inputs for Hexachlorobenzene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	6.2E+5	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	7.8E+5	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.4E-8	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	5.0E-3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	284.78	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.32E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	5.4E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	5.9E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2E+2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.0E+3	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.5E-2	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.9E-2	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	6.2E-3	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.3E-1	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	3.8E+5	Thomann et al., 1992
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	NA	
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	0.12	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.6	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	8E-4	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	4.6E-4	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-26. Chemical-Specific Inputs for Methylene chloride

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.7E+1	Calculated[1] (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.8E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	5.7E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.3E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	84.93	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	2.19E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.2E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	5.5E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	7.3	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	4.5E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.4E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	4.5E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	2.54	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	9.0	Howard et al., 1991[2]
K_n^{25}	Neutral Hydrolysis Rate Constant (y^{-1})	1E-3	Kollig, 1993
K_b^{25}	Base Second-order Rate Constant (M^{-1}Y^{-1})	0.60	Kollig, 1993
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	7.5E-3	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	6E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	4.7E-7	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	3	U.S. EPA, 1997a (HEAST)

NA = Not Available.

[1] K_{oc} value for analysis of the groundwater pathway was 8.51 cm^3/g.

[2] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-27. Chemical-Specific Inputs for Methyl ethyl ketone

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.9	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.9	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.25E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.23E+5	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	72.11	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	5.59E-5	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	8.1E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	9.8E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2E-1	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	8.7E-1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.7E+1	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	4.8E-8	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	1.5E-8	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.1E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	4.36E-1	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	36	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	6.0E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	1	U.S. EPA, 1998a (IRIS)

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-28. Chemical-Specific Inputs for Pentachlorophenol[1]

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	1.0E+5	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	1.2E+5	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	4.2E-8	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.0E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	266.34	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	2.4E-8	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	5.6E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	6.1E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant bio-transfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.5E+6	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	2.5E+2	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bio-concentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	4.4E-2	Calculated (U.S. EPA, 1993)
Ba_{beef}	Bio-transfer factor for beef (day/kg)	3.1E-3	Calculated (U.S. EPA, 1993)
Ba_{milk}	Bio-transfer factor for milk (day/kg)	9.8E-4	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.9E-1	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bio-accumulation Factor (L/kg)	6.29E+2	Thomann et al., 1992
BCF_{Fish}	Fish Bio-concentration factor (L/kg)	NA	
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.2E-1	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	3.0E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] Known to ionize under environmental conditions

Table C-29. Chemical-Specific Inputs for Phenol

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	2.9E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	3.0E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	3.6E-4	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	8.3E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	94.11	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	4.0E-7	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	8.2E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	9.1E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	5.3E+2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.2	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.4	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	7.6E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	2.4E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.7E-03	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	3.85	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	6.0E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-30. Chemical-Specific Inputs for Styrene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	7.8E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	8.7E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	8.1E-3	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	3.1E+2	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	104.15	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	2.8E-3	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.1E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2.7	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	6.4	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	.77	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.2E-5	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	6.9E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.4E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	55.0	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	2.0E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	1.0	U.S. EPA, 1998a (IRIS)

NA = Not Available.

Table C-31. Chemical-Specific Inputs for Tetrachloroethylene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	4.2E+02	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	4.7E+02	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.4E-2	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2E+02	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	165.83	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.84E-2	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.2E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	8.2E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	2.1E-1	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	4.3	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.1	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.2E-5	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	3.7E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.5E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	4.14E+1	Veith et al., 1980
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	0.7	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	5.2E-2	U.S. EPA, 1989b
RfD	Reference Dose (mg/kg/day)	1E-2	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	5.8E-7	U.S. EPA, 1989b
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-32. Chemical-Specific Inputs for Trichloroethylene

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	4.6E+2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	5.1E+2	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	9.67E-2	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.1E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	131.39	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	1.03E-2	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	7.9E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	9.1E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.2E-1	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	4.5	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.1	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.3E-5	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	4.1E-6	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	2.5E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	3.62E+1	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	0.7	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.1E-2	U.S. EPA, 1989b
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	1.7E-6	U.S. EPA, 1989b
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-33. Chemical-Specific Inputs for 2,4,5-Trichlorophenol

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	6.8E+3	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	7.9E+3	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	2.6E-5	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	1.2E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	197.45	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	4.33E-6	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	2.9E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	7.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.8E+4	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	3.1E+1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	.22	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	2.0E-4	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	6.3E-5	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	6.9E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	5.4E+2	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	1.0E-1	U.S. EPA, 1998a (IRIS)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-34. Chemical-Specific Inputs for 2,4,6-Trichlorophenol

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	4.3E+3	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	5.0E+3	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	3.2E-5	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	8.0E+2	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	197.45	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	7.8E-6	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	3.1E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	6.4E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	6.3E+3	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	22.0	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	.28	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.3E-4	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	4.0E-5	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	5.0E-2	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	2.19E+2	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.1E-2	U.S. EPA, 1998a (IRIS)
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	3.1E-6	U.S. EPA, 1998a (IRIS)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

Table C-35. Chemical-Specific Inputs for Vinyl acetate

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	5.2	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	5.37	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	1.19E-1	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2E+4	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	86.09	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	5.11E-4	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	8.5E-2	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	9.2E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	6.6E-2	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	9.3E-1	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.5E+1	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	1.3E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	4.3E-8	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	1.9E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bi-concentration factor (L/kg)	7.62E-1	Isnard et al., 1988
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	NA	
RfD	Reference Dose (mg/kg/day)	1	U.S. EPA, 1997a (HEAST)
URF	Unit Risk Factor (per µg/m^3)	NA	
RfC	Reference Concentration (mg/m^3)	2E-1	U.S. EPA, 1998a (IRIS)

NA = Not Available.

Table C-36. Chemical-Specific Inputs for Vinyl chloride

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1	Conservatively assumed to be 1 for volatile chemicals
K_{oc}	Soil Adsorbtion Coefficient (mL/g)	3E+1	Calculated (Di Toro et al., 1991)
K_{ow}	Octanol-water partition coefficient (unitless)	3.2E+1	U.S. EPA, 1996b (SCDM)
VP	Vapor Pressure (atm)	3.92	U.S. EPA, 1996b (SCDM)
Sol	Water solubility (mg/L)	2.76E+3	U.S. EPA, 1996b (SCDM)
MW	Molecular Weight (g/mol)	62.50	U.S. EPA, 1996b (SCDM)
H	Henry's Law Constant (atm-m^3/mol)	2.7E-2	U.S. EPA, 1996b (SCDM)
D_a	Diffusivity in air (cm^2/sec)	1.1E-1	U.S. EPA, 1994c
D_w	Diffusivity in water (cm^2/sec)	1.2E-5	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	8.2E-3	Calculated (U.S. EPA, 1993)
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/mL soil water])	1.3	Calculated (U.S. EPA, 1993)
Br	Plant-Soil Bioconcentration Factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.3	Calculated (U.S. EPA, 1993)
Ba_{beef}	Biotransfer factor for beef (day/kg)	7.9E-7	Calculated (U.S. EPA, 1993)
Ba_{milk}	Biotransfer factor for milk (day/kg)	2.5E-7	Calculated (U.S. EPA, 1993)
PC	Skin Permeability constant for water (cm/hr)	9.2E-3	Calculated (U.S. EPA, 1992a)
BAF_{Fish}	Fish Bioaccumulation Factor (L/kg)	NA	
BCF_{Fish}	Fish Bioconcentration factor (L/kg)	4.01	U.S. EPA, 1991
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c
ksg_F	Biodegradation Rate Constant (y^{-1})	1.4	Howard et al., 1991[1]
Health Benchmarks			
CSF	Cancer Slope Factor (per mg/kg/day)	1.9	U.S. EPA, 1997a (HEAST)
RfD	Reference Dose (mg/kg/day)	NA	
URF	Unit Risk Factor (per µg/m^3)	8.4E-5	U.S. EPA, 1997a (HEAST)
RfC	Reference Concentration (mg/m^3)	NA	

NA = Not Available.

[1] The soil biodegradation rate was estimated as ln2/soil half-life.

Table C-37. Chemical-Specific Inputs for 2,3,7,8-TCDD

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		5.5E-1	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)		2.7E+6	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)		4.4E+6	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)		9.7E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)		1.9E-5	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)		322	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)		1.6E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)		4.7E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)		8.0E-6	U.S. EPA, 1994c
Transfer Factors				
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])		6.1E+4	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])		5.2E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	leafy	5.6E-3	1
		forage	6E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)		7.0E-2	Ba_{milk} x 7[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)		1.0E-2	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)		9E-2	U.S. EPA, 1994b
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		6.0E-1	U.S. EPA, 1995
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		156,000	U.S. EPA, 1997a (HEAST)
RfD	Reference dose (mg/kg/d)		NA	
URF	Unit risk factor (per µg/m^3)		3.3E+1	U.S. EPA, 1998a (IRIS)
RfC	Reference concentration (mg/m^3)		NA	
$TEF_{H,M}$	Toxicity equivalency factor for humans		1	U.S. EPA, 1994b

NA = Not Available

[1] Calculated from an equation in Travis and Arms, 1988. Br for forage was inadvertently rounded to 6.0E-3, but does not have any appreciable effects.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-38. Chemical-Specific Inputs for 2,3,7,8-TCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	7.1E-1	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	2.1E+6	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	3.4E+6	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	1.2E-11	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	4.2E-4	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	306	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	8.6E-6	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm2/s)	4.8E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	8.1E+4	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	1.5E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	6.5E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	1.0E-2	Ba_{milk} x 3.3[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	3.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	9E-2	U.S. EPA 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-39. Chemical-Specific Inputs for 1,2,3,7,8-PeCDD

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	2.6E-1	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	2.7E+6	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	4.4E+6	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	1.2E-12	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.2E-4	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	356.4	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	2.6E-6	U.S. EPA, 1994a, b
Da	Diffusivity in air (cm^2/s)	4.5E-2	U.S. EPA, 1994a, b
Dw	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.2E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	3.9E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	5.6E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	6.0E-2	Ba_{milk} x 6[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	1.0E-2	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	9E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.5	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-40. Chemical-Specific Inputs for 1,2,3,7,8-PeCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	4.2E-1	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	3.8E+6	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	6.2E+6	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	3.6E-12	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	2.4E-4	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	340.4	U.S. EPA, 1994a, b
H	Henry’s law constant (atm-m^3/mol)	6.2E-6	U.S. EPA, 1994a, b
Da	Diffusivity in air (cm^2/s)	4.6E-2	U.S. EPA, 1994a, b
Dw	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.6E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	5.1E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	4.6E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	1.0E-2	Ba_{milk} x 5[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	2.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	9E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.05	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-41. Chemical-Specific Inputs for 2,3,4,7,8-PeCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	3.0E-1	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	5.1E+6	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	8.3E+6	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	4.3E-12	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	2.4E-4	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	340.4	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	6.2E-6	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.6E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g air])	4.6E+5	Lorber, 1995
RCF	Root concentration factor ([μg pollutant/g plant tissue FW]/[μg pollutant/g soil water])	3.1E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g soil])	3.9E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	5.0E-2	Ba_{milk} x 5.4[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	9.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	9E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.5	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-42. Chemical-Specific Inputs for 1,2,3,4,7,8-HxCDD

Parameter	**Definition**	**Value**	**Ref**
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	7E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	3.8E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	6.2E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	1.3E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	4.4E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	390.9	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	1.2E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.3E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	3.0E+4	U.S. EPA, 1994b
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.2E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	3.0E-2	Ba_{milk} x 5[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	6.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

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[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-43. Chemical-Specific Inputs for 1,2,3,6,7,8-HxCDD

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	4.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	1.2E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	2.0E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	4.7E-14	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	4.4E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	390.9	U.S. EPA, 1994a, b
H	Henry’s law constant (atm-m^3/mol)	1.2E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.3E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	1.3E+4	U.S. EPA, 1997b
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	3.0E-2	Ba_{milk} x 6[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	5.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-44. Chemical-Specific Inputs for 1,2,3,7,8,9-HxCDD

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	2.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	1.2E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	6.2E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	6.4E-14	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	4.4E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	390.9	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	1.2E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.3E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	1.3E+4	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	3.0E-2	Ba_{milk} x 5[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	6.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-45. Chemical-Specific Inputs for 1,2,3,4,7,8-HxCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	6.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	1.2E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	2.0E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	3.2E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	8.3E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	374.9	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	1.4E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.4E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	7.4E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	4.0E-2	Ba_{milk} x 5.4[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	7.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-46. Chemical-Specific Inputs for 1,2,3,6,7,8-HxCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	6.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	1.2E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	2.0E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	2.9E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.8E-5	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	374.9	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	6.1E-6	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.4E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	7.4E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	3.0E-2	Ba_{milk} x 5[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	6.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-47. Chemical-Specific Inputs for 1,2,3,7,8,9-HxCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	1.1E-1	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	1.2E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	2.0E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	3.7E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.3E-5	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	374.9	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	1.0E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.4E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	7.4E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	3.0E-2	Ba_{milk} x 5[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	6.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-48. Chemical-Specific Inputs for 2,3,4,6,7,8-HxCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	7.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	1.2E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	2.0E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	2.6E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.3E-5	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	374.9	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	1.0E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.4E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	7.4E+3	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	2.3E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	3.0E-2	Ba_{milk} x 6[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	5.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	4E-2	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.1	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-49. Chemical-Specific Inputs for 1,2,3,4,6,7,8-HpCDD

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	2.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	9.8E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	1.6E+8	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	4.2E-14	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	2.4E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	425.3	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	7.5E-6	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.1E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	3.5E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	4.4E+4	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	7.1E-4	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	6E-3	Ba_{milk} x 6[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	1E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	5E-3	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.01	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-50. Chemical-Specific Inputs for 1,2,3,4,6,7,8-HpCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	4.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	4.9E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	7.9E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	1.8E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.4E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	409.3	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	5.3E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.2E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.4E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	3.7E+4	U.S. EPA, 1994b
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.1E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	6.0E-3	Ba_{milk} x 6[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	1.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	5E-3	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.01	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-51. Chemical-Specific Inputs for 1,2,3,4,7,8,9-HpCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	3.0E-2	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	4.9E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	7.9E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	1.4E-13	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.4E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	409.3	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	5.3E-5	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.2E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	4.4E+5	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	3.7E+4	U.S. EPA, 1994b
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	1.1E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	1.0E-2	Ba_{milk} x 3.3[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	3.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	5E-3	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.01	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-52. Chemical-Specific Inputs for 1,2,3,4,5,7,8,9-OCDD

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	2.0E-4	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	2.4E+7	U.S. EPA, 1994a, b
K_{ow}	Octanol-water partition coefficient (unitless)	3.9E+7	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	1.1E-15	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	7.4E-8	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	460.8	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	7.0E-9	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	3.9E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g air])	8.6E+6	Lorber, 1995
RCF	Root concentration factor ([μg pollutant/g plant tissue FW]/[μg pollutant/g soil water])	6.2E+4	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g soil])	1.6E-3	1
Ba_{beef}	Biotransfer factor for beef (d/kg)	8.0E-3	Ba_{milk} x 8[2]
Ba_{milk}	Biotransfer factor for milk (d/kg)	1.0E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	1E-4	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.001	U.S. EPA, 1994b

[1] Calculated from an equation in Travis and Arms, 1988.

[2] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio for this analysis was incorrectly obtained from another project. The correct ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-53. Chemical-Specific Inputs for 1,2,3,4,6,7,8,9-OCDF

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	2.0E-3	U.S. EPA, 1994a, b
K_{oc}	Soil adsorption coefficient (mL/g)	3.9E+8	U.S. EPA, 1994a, b[1]
K_{ow}	Octanol-water partition coefficient (unitless)	6.3E+8	U.S. EPA, 1994a, b
VP	Vapor pressure (atm)	4.9E-15	U.S. EPA, 1994a, b
Sol	Water solubility (mg/L)	1.2E-6	U.S. EPA, 1994a, b
MW	Molecular weight (g/mol)	444.8	U.S. EPA, 1994a, b
H	Henry's law constant (atm-m^3/mol)	1.9E-6	U.S. EPA, 1994a, b
D_a	Diffusivity in air (cm^2/s)	4.0E-2	U.S. EPA, 1994a, b
D_w	Diffusivity in water (cm^2/s)	8.0E-6	U.S. EPA, 1994c
Transfer Factors			
Bv	Air-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g air])	1.3E+6	Lorber, 1995
RCF	Root concentration factor ([µg pollutant/g plant tissue FW]/[µg pollutant/g soil water])	1.8E+5	U.S. EPA, 1997c
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	3.2E-4	2
Ba_{beef}	Biotransfer factor for beef (d/kg)	5E-3	Ba_{milk} x 5.4[3]
Ba_{milk}	Biotransfer factor for milk (d/kg)	1E-3	U.S. EPA, 1995
BSAF	Fish biota to sediment accumulation factor (unitless)	1E-4	U.S. EPA, 1994b
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	6.0E-1	U.S. EPA, 1995
Health Benchmarks			
$TEF_{H,M}$	Toxicity equivalency factor for humans	0.001	U.S. EPA, 1994b

[1] K_{oc} value for analysis of the groundwater pathway was 4.8E+6 cm^3/g.

[2] Calculated from an equation in Travis and Arms, 1988.Pork biotransfer factor set equal to beef biotransfer factor.

[3] The Ba_{beef} for dioxin congeners was calculated from the Ba_{milk} and the ratio of percent beef fat to percent milk fat. The ratio is 5.4, that is the biotransfer factor for beef is 5.4 times higher than for milk.

Table C-54. Chemical-Specific Inputs for Arsenic

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		200	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		200	[1]
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		200	[2]
MW	Molecular Weight (g/mol)		74.92	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	0.008 0.036 0.06	U.S. EPA, 1992b U.S. EPA, 1992b U.S. EPA, 1992b
Ba_{beef}	Biotransfer factor for beef (d/kg)		0.002	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		6.0E-5	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		3.5	Stephan, 1993
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		1.5	U.S. EPA, 1998a (IRIS)
RfD	Reference dose (mg/kg/d)		0.0003	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per $\mu g/m^3$)		0.0043	U.S. EPA, 1998a (IRIS)
RfC	Reference concentration (mg/m^3)		NA	

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-55. Chemical-Specific Inputs for Barium

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		60	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		60	[1]
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		60	[2]
MW	Molecular Weight (g/mol)		137.33	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	0.015 0.15 0.15	Baes et al., 1984 Baes et al., 1984 Baes et al., 1984
Ba_{beef}	Biotransfer factor for beef (d/kg)		1.5E-4	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		3.5E-4	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		NA	
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		0.07	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per $\mu g/m^3$)		NA	
RfC	Reference concentration (mg/m^3)		0.0005	U.S. EPA, 1997a (HEAST)

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-56. Chemical-Specific Inputs for Cadmium

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		6.5	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		6.5	[1]
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		6.5	[2]
MW	Molecular Weight (g/mol)		112.41	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables	0.064	U.S. EPA, 1992b
		leafy vegetables	0.36	U.S. EPA, 1992b
		forage / silage	0.14	U.S. EPA, 1992b
Ba_{beef}	Biotransfer factor for beef (d/kg)		1.6E-4	U.S. EPA, 1995[3]
Ba_{milk}	Biotransfer factor for milk (d/kg)		0.0001	U.S. EPA, 1995[3]
BCF	Fish bioconcentration factor (L/kg)		270	Kumada, 1973
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		5E-4	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per $\mu g/m^3$)		0.0018	U.S. EPA, 1998a (IRIS)
RfC	Reference concentration (mg/m^3)		NA	

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

[3] The fraction of contaminant differed in the Chlorinated Aliphatics screening. The values should have been calculated using beef and dairy cattle consumption and uptake slopes from U.S. EPA, 1992b. The Ba beef value should have been 9.1E-4 d/kg and the Ba milk value should have been 7.6 E-5 d/kg.

Table C-57. Chemical-Specific Inputs for Chromium VI

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		850[1]	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		850	2
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		850	3
MW	Molecular Weight (g/mol)		52	U.S. EPA, 1996b (SCDM)
Transfer Factors				
B_r	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables	0.0045	Baes et al., 1984
		leafy vegetables	0.0075	Baes et al., 1984
		forage / silage	0.0075	Baes et al., 1984
Ba_{beef}	Biotransfer factor for beef (d/kg)		0.0055	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		0.0015	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		1	Stephan, 1993
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		0.003	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per $\mu g/m^3$)		0.012	U.S. EPA, 1998a (IRIS)
RfC	Reference concentration (mg/m^3)		.0001[4]	U.S. EPA, 1998a (IRIS)

NA = Not Available.

[1] Value cited is for chromium, not chromium VI.

[2] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[3] The Kd value for soil was used to approximate the Kd value for bottom sediment.

[4] RFC for Chromium (VI) particulates.

Table C-58. Chemical-Specific Inputs for Cobalt

Parameter	**Definition**		**Value**	**Ref**
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		45	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		45	1
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		45	2
MW	Molecular Weight (g/mol)		58.93	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	7.0E-5 2.0E-2 2.0E-2	Baes et al., 1984 Baes et al., 1984 Baes et al., 1984
Ba_{beef}	Biotransfer factor for beef (d/kg)		2.0E-2	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		2.0E-3	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		NA	
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)[1]		6.0E-2	U.S. EPA NCEA[3]
URF	Unit risk factor (per µg/m^3)		NA	
RfC	Reference concentration (mg/m^3)		NA	

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

[3] Provisional value - Risk Assessment paper by EPA’s National Center for Environmental Assessment.

Table C-59. Chemical-Specific Inputs for Manganese

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		65	Baes et al., 1994
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		65	1
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		65	2
MW	Molecular Weight (g/mol)		54.94	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([μg pollutant/g plant tissue DW]/[μg pollutant/g soil])	root vegetables	5.0E-2	Baes et al., 1984
		leafy vegetables	2.5E-1	Baes et al., 1984
		forage / silage	2.5E-1	Baes et al., 1984
Ba_{beef}	Biotransfer factor for beef (d/kg)		4.0E-4	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		3.5E-4	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		NA	
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		1.4E-1	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per μg/m^3)		NA	
RfC	Reference concentration (mg/m^3)		5.0E-5	U.S. EPA, 1998a (IRIS)

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-60. Chemical-Specific Inputs for Molybdenum

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		20	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		20	1
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		20	2
MW	Molecular Weight (g/mol)		95.94	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	6.0E-2 2.5E-1 8.5E-1	U.S. EPA, 1992b U.S. EPA, 1992b U.S. EPA, 1992b
Ba_{beef}	Biotransfer factor for beef (d/kg)		6.0E-3	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		1.5E-3	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		NA	
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997a
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		5E-3	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per µg/m^3)		NA	
RfC	Reference concentration (mg/m^3)		NA	

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-61. Chemical-Specific Inputs for Nickel

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		150	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		150	1
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		150	2
MW	Molecular Weight (g/mol)		58.69	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables	0.008	U.S. EPA, 1992b
		leafy vegetables	0.032	U.S. EPA, 1992b
		forage / silage	0.11[3]	U.S. EPA, 1992b
Ba_{beef}	Biotransfer factor for beef (d/kg)		0.006	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		0.001	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		0.8	Stephan, 1993
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		0.02[4]	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per µg/m^3)		2.4E-4[5]	U.S. EPA, 1998a (IRIS)
RfC	Reference concentration (mg/m^3)		NA	

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

[3] Only four studies (field studies) were used in deriving this value.

[4] RfD is for Nickel soluble salts.

[5] URF is for Nickel refinery dust.

Table C-62. Chemical-Specific Inputs for Vanadium

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		1000	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		1000	1
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		1000	2
MW	Molecular Weight (g/mol)		50.94	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	3.0E-3 5.5E-3 5.5E-3	Baes et al., 1984 Baes et al., 1984 Baes et al., 1984
Ba_{beef}	Biotransfer factor for beef (d/kg)		0.0025	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		0.002[3]	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		NA	
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		0.007	U.S. EPA, 1997a (HEAST)
URF	Unit risk factor (per µg/m^3)		NA	
RfC	Reference concentration (mg/m^3)		NA	

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

[3] Copy of Baes et al., 1984 was blurred; the original print was obtained to compare the values. The value should have been 2E-5.

Table C-63. Chemical-Specific Inputs for Zinc

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		40	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		40	1
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		40	2
MW	Molecular Weight (g/mol)		65.38	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables	0.044	U.S. EPA, 1992b
		leafy vegetables	0.25	U.S. EPA, 1992b
		forage / silage	0.096	U.S. EPA, 1992b
Ba_{beef}	Biotransfer factor for beef (d/kg)		1.2E-4	U.S. EPA, 1995[3]
Ba_{milk}	Biotransfer factor for milk (d/kg)		3.0E-5	U.S. EPA, 1995[3]
BCF	Fish bioconcentration factor (L/kg)		4.4	Stephan, 1993
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		0.3	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per $\mu g/m^3$)		NA	
RfC	Reference concentration (mg/m^3)		9.0E-4	CalEPA, 1997

NA = Not Available.

[1] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[2] The Kd value for soil was used to approximate the Kd value for bottom sediment.

[3] The fraction of contaminant differed in the Chlorinated Aliphatics screening. The values should have been calculated using beef and dairy cattle consumption and uptake slopes from U.S. EPA, 1992b. The Ba beef value should have been 6.8E-4 d/kg and the Ba milk value should have been 3.8E-4 d/kg.

Table C-64. Chemical-Specific Inputs for Aluminum[1]

Parameter	Definition	Value	Ref
Chemical/Physical Properties			
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)	0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)	1500	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)	1500	2
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)	1500	3
MW	Molecular Weight (g/mol)	26.98	U.S. EPA, 1996b (SCDM)
Other Parameters			
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)	0.6	U.S. EPA, 1997c

[1] Health benchmarks are not available.
[2] The Kd value for soil was used to approximate the Kd value for suspended sediment.
[3] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-65. Chemical-Specific Inputs for Copper[1]

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		35	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		35	2
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		35	3
MW	Molecular Weight (g/mol)		63.55	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	0.25 0.4 0.4	U.S. EPA, 1992b U.S. EPA, 1992b U.S. EPA, 1992b
Ba_{beef}	Biotransfer factor for beef (d/kg)		1.0E-2	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		1.5E-3	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		0	Stephan, 1993
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c

NA = Not Available.

[1] Health benchmarks are not available.

[2] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[3] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-66. Chemical-Specific Inputs for Lead[1]

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	Not assumed to volatilize
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		900	Baes et al., 1984
Kd_{sw}	Suspended sediment-surface water partition coefficient (L/kg)		900	2
Kd_{bs}	Bottom sediment-sediment pore water partition coefficient (L/kg)		900	3
MW	Molecular Weight (g/mol)		207.2	U.S. EPA, 1996b (SCDM)
Transfer Factors				
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	9.0E-3 1.3E-5 1.3E-5	Baes et al., 1984 Baes et al., 1984 Baes et al., 1984
Ba_{beef}	Biotransfer factor for beef (d/kg)		3.0E-4	Baes et al., 1984
Ba_{milk}	Biotransfer factor for milk (d/kg)		2.5E-4	Baes et al., 1984
BCF	Fish bioconcentration factor (L/kg)		4.6E+1	Stephan, 1993
BAF	Fish bioaccumulation factor (L/kg)		NA	
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997c

NA = Not Available.

[1] Health benchmarks are not available.

[2] The Kd value for soil was used to approximate the Kd value for suspended sediment.

[3] The Kd value for soil was used to approximate the Kd value for bottom sediment.

Table C-67. Chemical-Specific Inputs for Mercury-methyl

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		0	See Appendix D.3
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		NAP	[1]
MW	Molecular Weight (g/mol)		NAP	[1]
Transfer Factors				
Bv	Air-to-plant biotransfer factor ([ug pollutant/g plant tissue]/[ug pollutant/g air])	leafy vegetables forage/silage/grain	2.4E+3 5.0E+3	U.S. EPA, 1998b[2] U.S. EPA, 1997b
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	0.15 0.017 0	U.S. EPA, 1997b U.S. EPA, 1998b[2] U.S. EPA, 1997b
Ba_{beef}	Biotransfer factor for beef (d/kg)		2.0E-2	U.S. EPA, 1997b
Ba_{milk}	Biotransfer factor for milk (d/kg)		2.0E-2	U.S. EPA, 1997b
BCF	Fish bioconcentration factor (L/kg)		NA	
BAF	Fish bioaccumulation factor (L/kg)	Trophic Level 3 Trophic Level 4 Composite[3]	1.6E+6 6.8E+6 4.9E+6	U.S. EPA, 1997b U.S. EPA, 1997b U.S. EPA, 1997b
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		NA	1
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		1.0E-4	U.S. EPA, 1998a (IRIS)
URF	Unit risk factor (per µg/m^3)		NA	
RfC	Reference concentration (mg/m^3)		NA	

NAP = Not Applicable.
NA = Not Available.

[1] The values are known but are not used in the model.

[2] The values in U.S. EPA, 1998b Combustor Document was used. The Combustor Document was based on the Mercury Report to Congress, 1997.

[3] Composite value based on ingestion of 36% trophic level 3 fish and 64% trophic level 4 fish, as presented in the 1996 Exposure Factors Handbook (U.S. EPA, 1996a).

Table C-68. Chemical-Specific Inputs for Mercury-elemental

Parameter	Definition		Value	Ref
Chemical/Physical Properties				
F_v	Fraction of pollutant air concentration present in the vapor phase (dimensionless)		1	See Appendix D.3
Kd_s	Soil-water partition coefficient (mL/g or L/kg)		1.0E+3	U.S. EPA, 1997b
VP	Vapor Pressure (atm)		2.6E-6	U.S. EPA, 1989a
MW	Molecular Weight (g/mol)		201	U.S. EPA, 1996b (SCDM)
H	Henry’s Law Constant (atm-m^3/mol)		7.1E-3	U.S. EPA, 1997b
D_a	Diffusivity in air (cm^2/sec)		5.5E-2	U.S. EPA, 1997b
D_w	Diffusivity in water (cm^2/sec)		8.0E-6	U.S. EPA, 1994c
Transfer Factors				
Bv	Air-to-plant biotransfer factor ([ug pollutant/g plant tissue]/[ug pollutant/g air])	leafy vegetables forage/silage/grain	NAP	[1]
Br	Soil-to-plant biotransfer factor ([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])	root vegetables leafy vegetables forage / silage	NAP	[1]
Ba_{beef}	Biotransfer factor for beef (d/kg)		NAP	[1]
Ba_{milk}	Biotransfer factor for milk (d/kg)		NAP	[1]
BCF	Fish bioconcentration factor (L/kg)		NAP	[1]
BAF	Fish bioaccumulation factor (L/kg) - Trophic Level 4		NAP	[1]
Other Parameters				
F_w	Fraction of wet deposition that adheres to plant surfaces (dimensionless)		0.6	U.S. EPA, 1997b
Health Benchmarks				
CSF	Cancer slope factor (per mg/kg/d)		NA	
RfD	Reference dose (mg/kg/d)		NA	
URF	Unit risk factor (per µg/m^3)		NA	
RfC	Reference concentration (mg/m^3)		3.0E-4	U.S. EPA, 1998a (IRIS)

NAP = Not Applicable.
NA = Not Available.

[1] The values are known but are not used in the model.

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Appendix D.1

Partitioning Models

Appendix D.1

Partitioning Models

This appendix describes the partitioning models that were used to estimate contaminant losses from the following waste management scenarios.

- EDC/VCM Sludge managed in On-site Land Treatment Unit (LTU);
- EDC/VCM Sludge managed in Off-site Municipal Landfill; and
- Methyl Chloride Sludge managed in On-site Nonhazardous Waste Landfill.

The general partitioning model is first described and then the specific application of the partitioning model to the LTU and landfills is discussed.

Partitioning Model

A partitioning model is a spreadsheet calculation model that estimates the contaminant losses from contaminated soils due to volatilization, leaching, rainwater runoff, and chemical transformation (e.g., biodegradation and hydrolysis). The model assumes linear partitioning, first order rate losses, and uses a finite difference (numerical) integration approach to solve the mass balance equations. The model is limited in that it does not consider concentration profiles within the contaminated soil and it does not allow for differences in the permeability (density, void fraction, and organic content) within or between different soil layers.

The model calculates the average annual soil concentration, the annual mass of contaminant volatilized, and the annual mass of contaminant removed in the leachate.

Model Theory

Equilibrium Partitioning

The total concentration of contaminant in the soil can be expressed as the sum of the masses of contaminant adsorbed on the soil or waste particles, dissolved in the liquid, and in the air spaces divided by the total mass of contaminated soil as follows:

$$C_T = C_s + (\theta_w \, C_w/\rho_b) + (\theta_a \, C_a/\rho_b) \qquad (1)$$

where

C_T = total contaminant concentration (mg/kg = g/Mg)
C_s = concentration of contaminant adsorbed on soil (mg/kg = g/Mg)
θ_w = water-filled soil porosity (m^3_{water}/m^3_{soil})
C_w = concentration of contaminant in liquid ($\mu g/cm^3 = g/m^3$)
ρ_b = soil dry bulk density ($g/cm^3 = Mg/m^3$)
θ_a = air-filled soil porosity (m^3_{air}/m^3_{soil})

C_a = concentration of contaminant in air ($\mu g/cm^3 = g/m^3$).

The adsorbed contaminant concentration is assumed to be linearly related to the liquid phase concentration as follows:

$$C_s = K_d\, C_w \qquad (2)$$

where

C_s = concentration of contaminant adsorbed on soil (mg/kg = g/Mg)
K_d = soil-water partition coefficient ($cm^3/g = m^3/Mg$) = $K_{oc}\, f_{oc}$ for organic compounds
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g)
C_w = concentration of contaminant in liquid ($\mu g/cm^3 = g/m^3$).

The contaminant concentration in the vapor phase is assumed to be linearly related to the liquid phase concentration as follows:

$$C_a = H'\, C_w \qquad (3)$$

where

C_a = concentration of contaminant in air ($\mu g/cm^3 = g/m^3$)
H' = dimensionless Henry's Law constant = 41 × H
H = Henry's Law constant at 25 °C ($atm\text{-}m^3/mol$)
C_w = concentration of contaminant in liquid ($\mu g/cm^3 = g/m^3$).

Equations 2 and 3 assume linear equilibrium partitioning between the adsorbed contaminant, the dissolved contaminant and the volatilized contaminant. Combining Equations 1, 2, and 3 yields:

$$C_T = C_s\,[1 + \theta_w/(K_d\rho_b) + \theta_a\, H'/(K_d\rho_b)]. \qquad (4)$$

The total contaminant concentration, C_T, represents the measured soil concentration. However, it is the adsorbed soil concentration that is needed to calculate the equilibrium liquid and air contaminant concentrations (Equations 2 and 3). Equation 4 can be rearranged to calculate the adsorbed soil contaminant concentration given the total contaminant concentration as follows:

$$C_s = \frac{C_T\, K_d\, \rho_b}{(K_d\, \rho_b + \theta_w + \theta_a\, H')}\ . \qquad (5)$$

Overall Mass Balance

For a constant volume system assuming first-order rate loss mechanisms, the mass balance can be expressed as:

$$(\delta C_T / \delta t) = -(k_{app,air} + k_{app,leach} + k_{app,runoff} + k_{app,chemt})\, C_T \qquad (6)$$

where

$k_{app,air}$ = the apparent first order rate constant for volatilization, 1/sec
$k_{app,leach}$ = the apparent first order rate constant for leaching, 1/sec
$k_{app,runoff}$ = the apparent first order rate constant for rain runoff, 1/sec
$k_{app,chemt}$ = the apparent first order rate constant for chemical transformation, 1/sec
C_T = total contaminant concentration (mg/kg = g/Mg).

For small enough time steps (time steps in which C_T changes only a few percent), Equation 6 can be approximated as follows:

$$(M_{s,t+\Delta t} - M_{s,t})/(\Delta t) = -(k_{app,air} + k_{app,leach} + k_{app,runoff} + k_{app,chemt})\, M_{s,t} \qquad (7)$$

or

$$\Delta M_{tot} = \Delta M_{air} + \Delta M_{leach} + \Delta M_{runoff} + \Delta M_{chemt} \qquad (8)$$

where

$M_{s,t+\Delta t}$ = mass of contaminant in soil at time $t+\Delta t$ (g)
$M_{s,t}$ = mass of contaminant in soil at time t (g)
Δt = time step of calculation (sec)
$k_{app,air}$ = the apparent first order rate constant for volatilization (1/sec)
$k_{app,leach}$ = the apparent first order rate constant for leaching (1/sec)
$k_{app,runoff}$ = the apparent first order rate constant for rain runoff (1/sec)
ΔM_{tot} = total mass of contaminant removed from soil over time step (g) = $M_{s,t} - M_{s,t+\Delta t}$
ΔM_{air} = mass of contaminant lost over time step due to volatilization (g)
ΔM_{leach} = mass of contaminant lost over time step due to leaching (g)
ΔM_{runoff} = mass of contaminant lost over time step due to runoff (g)
ΔM_{chemt} = mass of contaminant lost over time step due to chemical transformation (g).

Due to the simplified nature of the numerical integration used, any number of competing loss mechanisms can be included in the model as each of the loss mechanisms can be evaluated separately and then summed together.

Loss to Atmosphere

The primary mechanism of contaminant loss to the atmosphere is the diffusion of volatilized contaminant to the soil surface. During periods of evaporation, the flux of water vapor enhances contaminant transport to the soil surface. Consequently, the total contaminant flux to the atmosphere is:

$$J_{air,t} = J_{vol,t} + J_{evaptr,t} \qquad (9)$$

where

$J_{vol,t}$ = contaminant flux to the atmosphere due to diffusion (g/m^2-s)
$J_{evaptr,t}$ = contaminant flux to the atmosphere due to evaporative transport (g/m^2-s).

The total mass loss to the air can be calculated as follows:

$$\Delta M_{air} = (J_{evaptr,t} + J_{vol,t})(A \Delta t). \tag{10}$$

where

$J_{evaptr,t}$ = contaminant flux to the atmosphere due to evaporative transport (g/m^2-s)
$J_{vol,t}$ = contaminant flux to the atmosphere due to diffusion (g/m^2-s)
A = area of contaminant source (m^2)
Δt = time step of calculation (sec).

The contaminant flux to the atmosphere terms are estimated using the following equations based on whether the contaminated soil layer is in direct contact with the atmosphere ("no soil cover") or buried beneath a layer of uncontaminated soil ("soil cover").

Emissions With No Soil Cover

Assuming that there is no soil cover and no stagnant boundary air layer at the ground surface, the Jury et al. (1990) simplified finite source model for diffusional volatilization can be written as:

$$J_{vol,t} = C_T \left(\frac{0.01\ D_A}{\pi t} \right)^{½} \left[1 - \exp\left(\frac{-d_s^2}{0.04\ D_A\ t} \right) \right] \tag{11}$$

where

C_T = total contaminant concentration (mg/kg = g/Mg)
D_A = apparent diffusivity (cm^2/sec)
π = 3.14
t = time (sec)
d_s = depth of uniform soil contamination at t=0, i.e., depth of daily addition (m).

and

$$D_A = \left[\frac{\left(\theta_a^{\frac{10}{3}}\ D_i\ H' + \theta_w^{\frac{10}{3}} D_w \right)}{n^2\ (\rho_b\ K_d + \theta_w + \theta_a\ H')} \right] \tag{12}$$

where

θ_a = air-filled soil porosity (m^3_{air}/m^3_{soil})
D_i = diffusivity in air (cm^2/sec)

H' = dimensionless Henry's Law constant = 41 × H
H = Henry's Law constant at 25 °C (atm-m^3/mol)
θ_w = water-filled soil porosity (m^3_{water}/m^3_{soil})
D_w = diffusivity in water (cm^2/sec)
n = total soil porosity (L_{pore}/L_{soil}) = $1 - (\rho_b/\rho_s)$
ρ_b = soil dry bulk density ($g/cm^3 = Mg/m^3$)
ρ_s = soil particle density (g/cm^3)
K_d = soil-water partition coefficient ($cm^3/g = m^3/Mg$) = $K_{oc}\, f_{oc}$ for organic compounds
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g).

As discussed in Jury et al. (1984), volatilization with evaporation is a complex problem, but evaporation always increased the overall volatilization rate. Jury et al. (1984) presents an equation for the convection of contaminants caused by the flux of water in the soil. The convective volatilization flux caused by evaporation is then calculated by isolating the first half of the overall volatilization flux equation (Jury et al., 1983), which can be written as follows:

$$J_{evaptr,t} = ½\ C_T\ \rho_b\ (0.01\ V_E) \left[erfc\left(\frac{V_E\ t}{(4\ D_A\ t)^{½}} \right) - erfc\left(\frac{(100\ d_s + V_E\ t)}{(4\ D_A\ t)^{½}} \right) \right] \qquad (13)$$

where

C_T = total contaminant concentration (mg/kg = g/Mg)
ρ_b = soil dry bulk density ($g/cm^3 = Mg/m^3$)
V_E = evaporative convective velocity (cm/sec)
erfc(x) = complementary error function;
t = time (sec)
D_A = apparent diffusivity (cm^2/sec)
d_s = depth of uniform soil contamination at t=0 (m);

and

$$V_E = \left(\frac{-E}{(365 \times 24 \times 3600) \times (\rho_b\ K_d + \theta_w + \theta_a\ H')} \right) \qquad (14)$$

where

E = average annual evaporation rate (cm/yr)
ρ_b = soil dry bulk density ($g/cm^3 = Mg/m^3$)
K_d = soil-water partition coefficient ($cm^3/g = m^3/Mg$) = $K_{oc}\, f_{oc}$ for organic compounds
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g)
θ_w = water-filled soil porosity (m^3_{water}/m^3_{soil})
θ_a = air-filled soil porosity (m^3_{air}/m^3_{soil})
H' = dimensionless Henry's Law constant = 41 × H

H = Henry's Law constant at 25 °C (atm-m^3/mol)

[Note: the minus sign is introduced because upward movement is in the negative direction.]

Mass Lost Via Leaching

The mass flux loss of a contaminant due to leaching is estimated by assuming the leachate is in equilibrium with the soil (i.e., Equation 2 applies).

$$J_{leach,t} = \frac{C_T\ \rho_b\ (0.01\ V_L)}{(\rho_b\ K_d + \theta_w + \theta_a\ H')} \qquad (15)$$

where

$J_{leach,t}$ = contaminant flux in leachate at time t, g/m^2-s
C_T = total contaminant concentration (mg/kg = g/Mg)
ρ_b = soil dry bulk density (g/cm^3 = Mg/m^3)
V_L = $(P + I - R - E)/(365 \times 24 \times 3600]$ = leachate rate (cm/sec)
P = annual average precipitation rate (cm/yr)
I = annual average irrigation rate (cm/yr)
R = annual average runoff rate (cm/yr)
E = average annual evaporation rate (cm/yr)
K_d = soil-water partition coefficient (cm^3/g = m^3/Mg) = $K_{oc}\ f_{oc}$ for organic compounds
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g)
θ_w = water-filled soil porosity (m^3_{water}/m^3_{soil})
θ_a = air-filled soil porosity (m^3_{air}/m^3_{soil})
H' = dimensionless Henry's Law constant = $41 \times H$
H = Henry's Law constant at 25 °C (atm-m^3/mol)

In the same fashion that the air fluxes were converted a mass loss, the leaching flux rate can be converted to a mass loss as follows:

$$\triangle M_{leach} = (J_{leach,t})(A\triangle t). \qquad (16)$$

Loss Due to Runoff

The equation describing the mass flux loss of a contaminant due to runoff is nearly identical to Equation 15, because the runoff is also assumed to be in equilibrium with the contaminated soil. Consequently, the total mass rate of contaminant loss due to runoff is:

$$J_{runoff,t} = \frac{C_T\ \rho_b\ (0.01\ V_R)}{(\rho_b\ K_d + \theta_w + \theta_a\ H')} \qquad (17)$$

where

$J_{runoff,t}$ = contaminant run-off rate at time t (g/m^2-s)
C_T = total contaminant concentration (mg/kg = g/Mg)
ρ_b = soil dry bulk density ($g/cm^3 = Mg/m^3$)
V_R = $R/(365 \times 24 \times 3600]$ = runoff rate (cm/sec)
K_d = soil-water partition coefficient ($cm^3/g = m^3/Mg$) = $K_{oc}\ f_{oc}$ for organic compounds
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g)
θ_w = water-filled soil porosity (m^3_{water}/m^3_{soil})
θ_a = air-filled soil porosity (m^3_{air}/m^3_{soil})
H' = dimensionless Henry's Law constant = $41 \times H$
H = Henry's Law constant at 25 °C (atm-m^3/mol)

Then,

$$\Delta M_{runoff} = (J_{runoff,t})(A \Delta t). \tag{18}$$

Loss Due to Chemical Transformation

Chemical transformation (for example, biodegradation and hydrolysis) rates were imputed from reported soil half-lives. The soil half life was used to calculate an overall first order rate constant that included all loss mechanisms. Then the total mass loss predicted from this overall first order rate constant was calculated as follows:

$$\Delta M_{tot} = M_{s,t}\ [1 - \exp(-\ k_{app,overall}\ \Delta t)] \tag{19}$$

where

ΔM_{tot} = total mass of contaminant loss from the system (g)
$M_{s,t}$ = mass of contaminant in soil at time t (g)
$k_{app,overall}$ = the overall apparent first order rate constant (1/sec)
Δt = time step of calculation (sec)

If ΔM_{tot} exceeds the mass losses from volatilization, leaching and run-off, then the additional mass loss was attributed to (biodegradation+hydrolysis). If the volatilization, leaching and run-off mass losses exceeded ΔM_{tot}, then the mass chemically transformed was set to zero.

Application of Model to LTU

Under this analysis, we assumed that the land treatment unit operates for 40 years with annual waste applications (i.e., one application per year). At the end of 40 years, the LTU ceases to receive EDC/VCM sludge, but it may potentially continue to release contaminants into the environment. Therefore, the model tracks the average annual soil concentration and the annual mass of contaminant volatilized for the 40 years of active use followed by a period of 40 years of inactive use (i.e., no additional waste applications).

Land treating often involves tilling the waste into the soil. We assumed that the EDC/VCM sludge is tilled to a depth of 0.2 m (U.S.EPA 1990). We also assumed that there were no runoff/runon controls in place at the land treatment unit to mitigate the release of sludge via runoff.

The total mass of contaminant applied to the soil during the first annual application can be calculated as follows:

$$M_{s,app} = (C_T\ Q_{app}) \times 1\text{-yr} \qquad (20)$$

where

$M_{s,app}$ = mass of contaminant in soil from waste application (g)
C_T = total contaminant concentration (mg/kg = g/Mg)
Q_{app} = annual waste application rate (Mg/yr).

After each time interval, the mass of constituent remaining in the soil is calculated. We assumed that the contaminant concentrations were uniform over the tilling depth at the beginning of each time interval. The model does not attempt to assess the temporal concentration profiles (as a function of depth). This assumption is reasonable for active land treatment units that are tilled regularly.

Mass additions to the system occur during waste application. The depth of material added during an application is generally negligible; however, some model scenarios could have significant waste material accumulation over forty years depending on the tilling depth, application rate, and other factors. As waste is sequentially added, and given a fixed tilling depth, a small layer of contaminated soil at the bottom of the land treatment unit will not be tilled in with the newly added waste. The thickness of this layer is equal to the effective thickness of the applied waste (i.e., the volume of the applied waste divided by the surface area of the unit). This layer at the bottom of the unit basically becomes "buried" with successive waste applications. The contaminant remaining in this buried soil is assumed to have negligible affect on the emissions and leachate losses and is effectively removed from the active land treatment unit during waste application. Consequently, the net mass of contaminant added to the land treatment unit, accounting for this "burial loss", at the start of Year 2 through Year 40 is:

$$M_{s,app} = C_T\ Q_{app}\ [1 - \{(Q_{app} \times 1\text{-yr})/(A\ \rho_b\ )\}/d_{till}] \times 1\text{-yr} \qquad (21)$$

where

$M_{s,app}$ = mass of contaminant in soil from waste application (g)
C_T = total contaminant concentration (mg/kg = g/Mg)
Q_{app} = annual waste application rate (Mg/yr)
A = area of contaminant source (m^2)
ρ_b = soil dry bulk density ($g/cm^3 = Mg/m^3$)
d_{till} = tilling depth = 0.2 m.

A quality assurance review of the model uncovered the fact that, for the LTU, the evaporation rate used in estimating the contaminant flux to the atmosphere due to evaporative transport was estimated as 70 percent of the location-specific precipitation rate (i.e., 102.3 cm/yr) rather than the location-specific evaporation rate of 73.7 cm/yr. This 30 percent increase in the evaporation rate is estimated to increase the evaporative flux by 30 percent. However, as the evaporative flux was generally about 20 percent of the overall air emissions (volatilization plus evaporative fluxes), the overall impact on the projected air emissions is approximately 6%. Consequently, the overall impact on the risk estimates will not be notable given the level of significant figures used in this analysis.

Application of Model to Landfills

Under this analysis, only the volatilization loses estimated with the model were considered in developing risk estimates. Risks posed by leaching were also considered as part of this assessment but Toxicity Characteristic Leaching Procedure (TCLP) data were evaluated rather than the model loss estimates for leaching. We assumed that aerobic biodegradation and hydrolysis would be negligible. We did not have sufficient data to model anaerobic biodegradation within the landfill. Therefore, the biodegradation and hydrolysis rates were set to zero in the model.

The model evaluates contaminant losses over three separate conditions. The first condition is the daily waste addition in which the waste is in direct contact with the atmosphere. The second condition is the active landfill cell in which the waste is covered by a thin "daily" cover. The third condition is the closed landfill cell in which the waste is covered by a thick landfill cap. The model tracks the average annual soil concentration and sums and tracks both the annual emissions and leaching rates for the user specified active life of the landfill (duration for which the landfill receives waste for disposal) followed by 40 years of inactive use (i.e., closed landfill). Under this analysis, two landfill scenarios were modeled.

- EDC/VCM Sludge Off-site Municipal Landfill - We assumed that EDC/VCM sludges are disposed in off-site unlined municipal landfills. Based on municipal solid waste management requirements (40 CFR Part 258), we assumed that the landfills are covered daily (every 12 hours) with soil, and are capped at the end of their active life, which is 30 years (30 years is the average active lifetime of municipal Subtitle D landfills based on a survey conducted by EPA [U.S.EPA 1988]). We assumed that the landfill continues to release contaminants into the environment for 40 years after it is closed.

- Methyl Chloride Sludge On-site Nonhazardous Waste Landfill - Review of the §3007 survey responses found that methyl chloride sludge is managed at a single facility in a landfill that is lined with a 24-inch clay liner and has a leachate collection system. We estimated that the landfill would have an active life of 90 years. We assumed that the landfill continues to release contaminants into the environment for 40 years after it is closed.

The waste added to the landfill was assumed to be homogeneous and temporally consistent. One landfill cell was assumed to be filled per year. The user inputs the annual waste quantity and the contaminant concentration of the waste of interest, the waste density, the dimensions of the entire landfill, and the life expectancy of the landfill. From this information, the dilution effect of the target waste being added to other waste in the landfill was calculated. The partitioning equations were applied in three distinct compartments to the landfill model. These included: the daily waste addition in which the waste is in direct contact with the atmosphere; the active landfill cell in which the waste is covered by a thin "daily" cover; and the closed landfill cell in which the waste is covered by a thick landfill cap.

Losses from the daily waste addition were calculated over the time period when the waste was first added to the landfill until another daily addition was added on top of the waste. The waste was assumed to be uncovered in the landfill for a user specified time (model runs were made using an uncovered duration of 12 hours). The dimensions of the daily waste addition were specified by the number of operating days and the number of "layers" used to fill the landfill cell. It was assumed that a daily waste addition was 2.5 feet deep and that there were 350 operating days per year. It was assumed that the entire first layer of the cell was filled, then the second layer was filled in the same order as the first layer, and so on. Once waste was added on top of a daily addition "cell", it was assumed that the losses from that "daily cell" are minimal. Assuming that there were seven waste layers, the time of exposure (i.e., time before more waste was added on top of the waste) for a given daily cell was, on average, 365/7 or 52 days. The total amount of contaminant emitted and leached over the 52 days was estimated by the model for a given daily quantity by adding losses from 12 hours of uncovered waste to the losses calculated for the covered daily cell. These emissions and leaching estimates were then multiplied by 350 (350 equal daily additions) to yield annual amounts of contaminant emitted and leached from the active landfill cell.

During the active life of the landfill, there was always one active landfill cell. However, the number of capped landfill cells increased sequentially until the entire landfill was filled. The losses from the capped cell are modeled over a 40 year period. The annual losses from this capped cell (closed or inactive landfill) simulation were then used to project the annual losses for the landfill. For example, in Year 1, there were losses from an active cell. In Year 2, there were losses from an active cell plus losses from the first year of a capped cell. In Year 3, there were losses from an active cell plus losses from both the first year losses of a (most recently) capped cell and the second year losses from a capped cell (the 2 year old capped cell), and so on. In this manner, the annual losses from the entire landfill were simulated from the annual losses of an active cell and a single capped cell.

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Appendix D.2

Overland Transport Models

Appendix D.2

Overland Transport Models

Methodology

The Universal Soil Loss Equation (USLE) is an empirical erosion model originally designed to estimate long-term average soil erosion losses to a nearby waterbody from an agricultural field having uniform slope, soil type, vegetative cover, and erosion-control practices. In the risk assessment to be conducted in support of the proposed listing decision, the USLE will be used to estimate the mass of soil lost per year per unit area from a land treatment unit (LTU) and deposited directly onto the adjacent receptor site. A fixed sediment delivery ratio was used to estimate the percentage of eroded soil that ultimately reached the receptor site. The quantity of soil eroded from the LTU and deposited directly on each receptor site (agricultural field, residential lot, home garden) will be estimated independently of soil eroded from the LTU and deposited into the nearest surface waterbody.

The USLE was modified to estimate soil erosion and overland transport of sediment from LTUs across intervening areas to nearby waterbodies by evaluating this process in an integrated setting (Beaulieu et al., 1996). Because the USLE equation estimates only soil erosion to waterbodies, the receptor location is considered to be located between the LTU and the waterbody. For the purposes of the analysis, the LTU, the receptor site, and the intervening area constitutes a discrete drainage subbasin with uniform characteristics. The soil erosion load from the subbasin to the waterbody is estimated using a distance-based sediment delivery ratio and the sediment not reaching the waterbody is considered to be deposited evenly over the area of the subbasin. Thus, using mass balance equations, contributions to the constituent concentrations of the waterbody and of the receptor soil may be estimated. The equations implementing the concept of the integrated setting are based on the following assumptions:

- The area of the management unit (LTU) and the area between the management unit and the nearest waterbody, including the receptor site, make up a discrete drainage subbasin.

- The sediment delivery ratio (SD_{SB}) and the soil loss rate per unit area are assumed to be constant for all areas within the subbasin.

- The amount of soil deposited onto the receptor site through soil erosion is estimated by assuming that the fraction of soil that does not reach the waterbody remains in the subbasin.

- The entire subbasin drainage system is assumed to be at steady-state. Consequently, steady-state soil concentrations for the different subareas (e.g., receptor site, surrounding area) can be calculated using a mass balance approach.

- The soils within the subbasin are assumed (on the average) to have the same soil properties (e.g., bulk density, soil moisture content).

- No contributions to constituent concentrations are assumed to occur from sources other than the LTU within the subbasin.

Soil Load from LTU to Receptor Site

The mass of eroded soil (soil load) from the LTU to the receptor site ($SL_{O,F}$) is a major input required to calculate the receptor site soil constituent concentration (C_F). The receptor site (residential plot, home garden, or agricultural field) soil concentrations are used to estimate risk through the soil ingestion pathway for all scenarios and through the food chain pathways (e.g., above-ground and below-ground produce) for the home gardener and farmer scenarios. Assuming that the probability that soil from the LTU is transported and deposited is equivalent for the intervening area and receptor site, the amount of contaminated soil that leaves the source area can be calculated by using a simple ratio of the area of concern to the total area for soil deposition:

$$DS_{0,F} = X_e \times A_s \times (1 - SD_{SB}) \times SF_{0,F} \tag{D-1}$$

where

$DS_{0,F}$ = soil delivery rate from source (LTU) to receptor (kg/yr)
X_e = unit soil loss rate from LTU ($kg/m^2/yr$)
A_S = area of the LTU (m^2)
SD_{SB} = sediment delivery ratio of the subbasin to the nearest waterbody (unitless)
$SF_{0,F}$ = deposition area scaling factor (m^2/m^2)
= ratio of the receiving field area to the entire area available for deposition
= $A_F/(A_S + A_{B/Surr} + A_F)$
A_F = area of the receptor site (m^2)
$A_{B/Surr}$ = area of the buffer and surrounding areas within the subbasin (m^2).

Total Constituent Load to Waterbody

The total load to the waterbody (L_T) is the sum of the constituent load via erosion (L_E) and the constituent load from pervious runoff (L_R). For this analysis, the total constituent load is assumed to originate exclusively from the drainage subbasin, that is, contributions from other subbasins within the watershed are not included. The total load to the waterbody is used to estimate risk to the fisher from the ingestion of contaminated fish. The estimation of L_E requires the calculation of a weighted average constituent concentration in subbasin soils based on the eroded soil contribution ($S_{c,erode}$), and the L_R term requires the calculation of a weighted average constituent concentration based on the pervious runoff contribution ($S_{c,run}$). The weighted average constituent concentration represents the effective subbasin soil concentration based on contributions from the three components of the subbasin: the source area (LTU), the receptor field area (garden, agricultural field), and the buffer/surrounding area (intervening area that is not part of the receptor field). The calculation of L_T requires constituent concentrations for each of the following areas within the subbasin: the LTU, the receptor site, and the buffer/surrounding area.

If we consider the erosion load (L_E) to the surface waterbody for each of these areas individually, the equation may be written as:

$$\begin{aligned} L_E = \; & [X_{e,SB} \times ER \times SD_{SB} \times A_0 \times C_0 \times (\frac{Kd_s \; BD}{\theta + Kd_s \; BD}) \times 0.001] \; + \\ & [X_{e,SB} \times ER \times SD_{SB} \times A_F \times C_F \times (\frac{Kd_s \; BD}{\theta + Kd_s \; BD}) \times 0.001] \; + \\ & [X_{e,SB} \times ER \times SD_{SB} \times A_{B/Surr} \times C_{B/Surr} \times (\frac{Kd_s \; BD}{\theta + Kd_s \; BD}) \times 0.001]] \end{aligned} \tag{D-2}$$

where

L_E = constituent load to subbasin due to erosion (g/yr)
$X_{e,SB}$ = unit soil loss in subbasin (kg/m^2/yr)
ER = enrichment ratio
SD_{SB} = sediment delivery ratio for subbasin
A_0 = area of source (m^2)
C_0 = constituent concentration at the source (mg/kg)
Kd_s = soil water partition coefficient (L/kg)
BD = bulk density of soil (g/cm^3)
θ = volumetric soil content of soil (cm^3/cm^3)
0.001 = unit conversion factor ([g/kg]/[mg/kg]).
A_F = area of receptor field (m^2)
C_F = constituent concentration in receptor site field (mg/kg)
$A_{B/Surr}$ = area of buffer and surrounding area (m^2)
$C_{B/Surr}$ = constituent concentration in buffer and surrounding area (mg/kg)

The enrichment ratio (ER) reflects the tendency for lighter soil particles to erode more easily than heavier particles (lighter soil particles have higher surface-area-to-volume ratios and are higher in organic matter content). Therefore, concentrations of organic constituents, which are a function of organic carbon content of sorbing media, would be expected to be higher in eroded soil then in in situ soil. This factor is generally assigned values in the range of 1 to 5. A value of 3 for organic contaminants and a value of 1 for metals would be reasonable first estimates (U.S. EPA 1994).

Alternatively, this equation can be written in terms of an average weighted soil concentration for the entire subbasin (including the LTU, the receptor field, and the buffer/surrounding area) that results in the same constituent load as a function of erosion and sediment delivery. The weighted average soil concentration ($S_{c,erode}$) term shown at the end of Equation D-3 reflects this modification:

$$L_E = [X_e \times ER \times SD_{SB} \times A_{SB} \times (\frac{Kd_s\ BD}{\theta + Kd_s\ BD}) \times 0.001] \times S_{c,erode} \tag{D-3}$$

where

SD_{SB} = sediment delivery ratio for subbasin
A_{SB} = area of entire subbasin (m^2)

L_T also requires the constituent load from pervious runoff (L_R). The L_R term is calculated using equation D-4.

$$L_R = R \times (A_{SB} - A_I) \times \frac{S_c,erode \times BD}{\theta + Kd_s \times BD} \times 0.01 \tag{D-4}$$

where

L_R = pervious surface runoff load (g/yr)
R = average annual surface runoff (cm/yr)
A_{SB} = area of entire subbasin (m^2)
A_I = impervious subbasin area receiving constituent deposition (m^2)
$S_{c,erode}$ = weighted average constituent concentration in total subbasin soils based on surface area (mg/kg)
BD = soil bulk density (g/cm^3)
θ = volumetric soil content of soil (cm^3/cm^3)
Kd_s = soil water partition coefficient (L/kg) or (cm^3/g)
0.01 = units conversion factor ($kg\text{-}cm^2/mg\text{-}m^2$).

Assuming that the ratio of pervious and impervious soils is the same for each of the designated areas, a correction for areas that do not erode (streets, rocks, etc.) can be added to Equation D-3 by replacing A_{SB} with A_{SB} - A_I , where A_I equals the total impervious area in the subbasin. Setting the L_R equal to each other in the previous two equations and solving for $S_{c,erode}$ yields:

$$S_{c,erode} = \frac{(X_{e,SB} \times A_s \times C_0 \times SD_{SB}) + (X_{e,SB} \times A_{B/Surr} \times C_{B/Surr} \times SD_{SB}) + (X_{e,SB} \times A_F \times C_F \times SD_{SB})}{X_e \times SD_{SB} \times A_{SB}} \qquad \text{(D-5)}$$

Equation D-5 accounts for differences in the sediment delivery ratios (SD), surface areas (A), and mixing depths (Z) for discrete areas of the subbasin (source, receptor field, and buffer/surrounding areas). Similarly, the weighted average for runoff losses (ksr) was derived using the areas for various subbasin components; however, different sediment delivery ratios were not required because soils in the area were considered to be similar and the slope was considered uniform. It was possible to generate simple area-based weighting factors because the rainfall runoff per unit area was assumed to be constant for the entire subbasin area.

Constituent Concentrations in Various Subbasin Components

The constituent concentrations for the LTU (C_0), receptor site field (C_F), the buffer and surrounding area ($C_{B/Surr}$) are required to solve $S_{c,erode}$. As suggested previously, a mass balance approach was used to calculate the constituent concentrations for all subbasin components. For the receptor site field, the mass balance equation is given by:

$$M_F\,(dC_F/dt) = [(C_0\,SL_{0,F}) + (M_F\,Ds_{(1),F})] + (SL_{B,F}\,C_{B/Surr}) - (M_F\,ks_F\,C_F) \qquad \text{(D-6)}$$

where

M_F = mass of the field (kg)
C_F = constituent concentration in the receptor site field (mg/kg)
$SL_{0,F}$ = soil load from source to the field (kg/yr)
$Ds_{(1),F}$ = air deposition rate from source to the field (mg/kg-yr)
$SL_{B,F}$ = soil load from buffer to the field (kg/yr)
ks_F = constituent loss rate coefficient for the field (per yr).

At steady state, this equation can be solved for the constituent concentration in the receptor site field as follows:

$$C_F = [(C_0\,SL_{0,F} + M_F\,Ds_{(1),F}) + (SL_{B,F}\,C_{B/Surr})] / (M_F\,ks_F) \qquad \text{(D-7)}$$

As with the constituent concentration in the receptor site field, the concentration in the buffer and surrounding area is given by:

$$M_{B/Surr}(dC_{B/Surr} / dt) = (SL_{0,B/surr}\ C_0) + [M_{B/Surr}\ (Ds_{(1),B/Surr} - ks_{B/Surr}\ C_{B/Surr})] \qquad \text{(D-8)}$$

where

$M_{B/Surr}$ = mass of the buffer and surrounding area (kg)
$C_{B/Surr}$ = constituent concentration in the buffer and surrounding area (mg/kg)
$SL_{0,B/Surr}$ = soil load from source to buffer/surrounding areas (kg/yr)
C_0 = soil constituent concentration at the source (mg/kg)
$Ds_{(1),B/Surr}$ = air deposition rate from source to buffer and surrounding area (mg/kg/yr)
$ks_{B/Surr}$ = constituent loss rate coefficient for the buffer/surrounding area (per/yr).

Summary

Contaminated particles are transported from the land treatment unit to receptor sites via air deposition as well as runoff/erosion. For the integrated setting analysis, mass balance was applied for each area of interest (e.g., buffer area between source and receptor site, receptor site, or surrounding area). Consequently, the respective air deposition value for each area of interest is included in the evaluation of the mass balance. The air deposition over the entire subbasin area was considered to be uniform and equal to the air deposition modeled for the receptor site. The equations and default input parameter values used to calculate receptor subbasin soil concentrations and waterbody concentrations for constituents of concern are presented in Appendices E and K, respectively.

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Appendix D.3

Air Models

Appendix D.3

Air Models

Estimation of Particulate Emissions

For the EDC/VCM sludge land treatment unit (LTU), EPA used equations documented in EPA's "Compilation of Air Pollutant Emission Factors (AP-42)" (U.S. EPA 1995a) to estimate particulate emissions resulting from wind erosion and tilling activities. Emissions from wind erosion were modeled for particulates that are 10 microns (PM10) or smaller because (1) this is the size range of respirable particulates that is of concern to us from the standpoint of evaluating inhalation risks and (2) the emission of larger particles is relatively insignificant from this process. Emissions from tilling activities were modeled for both smaller (PM10) and larger (PM30) particles size ranges.

Particulate emissions due to wind erosion were modeled assuming that the LTU was not covered by continuous vegetation or snow and that the surface soils have an unlimited reservoir of erodible surface particles. The factors for estimating emission of particles due to wind erosion and tilling were obtained from AP-42 (U.S. EPA 1995a). The Emissions Factor and Inventory Group (EFIG) of the Office of Air Quality Planning and Standards (OAQPS) develops and maintains emissions estimating tools to support the many activities of the Agency. AP-42 is the principal means by which EFIG documents the equations used to estimate emissions factors. These emissions factors relate the quantity of a pollutant released to the atmosphere with an activity associated with the release, for example, releases of soil particles through wind erosion:

$$E_{wind} = 0.036 \bullet (1 - V) \bullet \left(\frac{u}{u_t} \right)^3 \bullet f(x) \qquad \text{(D.3-1)}$$

where

E_{wind} = emissions of PM_{10} (respirable particulate matter) from wind erosion ($g/m^2/s$)
V = vegetative cover (fraction)
u = mean windspeed (m/s)
u_t = threshold windspeed (m/s)
$f(x)$ = function of roughness height.

This empirical equation estimates only the emission of respirable particulate matter (PM_{10}) from the site and is not applicable for the emission of larger particles. The emission of larger particles is not a factor due to wind erosion.

During tilling, particulate matter created from loosening and pulverizing the soils is released into the atmosphere as the soil is dropped to the surface. The emission factor used to estimate tilling emissions in this analysis is based on the factor presented in U.S. EPA (1995a):

$$E_{at} = 5.38 \bullet K_{at} \bullet S^{0.6} \bullet N_{op} \bullet CF \qquad \text{(D.3-2)}$$

where

E_{at} = emissions of soil (PM_{10} or PM_{30}) from tilling ($g/m^2/s$)
K_{at} = particle size multiplier to adjust results to PM_{10} or PM_{30} (unitless)
S = silt content of soil (%)
N_{op} = number of days of operations (d)
CF = conversion factor ($[d \bullet g \bullet ha]/[s \bullet kg \bullet m^2]$).

In this analysis, a silt content of 60 percent was applied for Plaquemine, LA which is the location modeled for the LTU waste management scenario.

CHEMDAT8: Volatile Emission Estimates from Wastewater

The EPA modeled vapor emissions from aerated biological wastewater treatment tanks using the CHEMDAT8 model (U.S. EPA 1994). The resulting emission estimates were used in conjunction with the dispersion modeling results to estimate constituent specific air concentrations and deposition rates.

Model Selection

Several factors were considered in selecting emission models for assessing the potential for contaminant release from wastewaters through volatilization. The ideal emission model would provide as accurate emission estimates as possible without underestimating the contaminant emissions. That is, the model(s) would provide accurate to slightly high (environmentally conservative) estimates of the potential for air emissions.

EPA’s CHEMDAT8 model was selected to estimate volatile emissions rates from the wastewater tanks. The CHEMDAT8 model was originally developed in projects funded by EPA's Office of Research and Development (ORD) and Office of Air Quality Planning and Standards (OAQPS) to support National Emission Standards for Hazardous Air Pollutants (NESHAPs) from sources such as tanks, surface impoundments, landfills, wastepiles, and land application units for a variety of industry categories including chemical manufacturers, pulp and paper manufacturing, and petroleum refining. It also has been used to support the emissions standards for hazardous waste treatment, storage and disposal facilities regulated under Subpart

C rules of the Resource Conservation and Recovery Act (RCRA), as amended in 1984. The CHEMDAT8 model is publicly available and has undergone extensive review by both EPA and industry representatives. The CHEMDAT8 spreadsheet model and model documentation may be downloaded at no charge from EPA's web page (http://www.epa.gov/ttn/chief/software.html).

The CHEMDAT8 model considers most of the competing removal pathways that might limit air emissions, including adsorption, hydrolysis, and biodegradation. Adsorption is the tendency of a chemical or liquid media to attach or bind to the surface or fill the pores of particles in the waste and therefore limit volatilization into the air. Biodegradation is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by organisms in the waste. Similarly, hydrolysis is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by reaction with water. Chemicals that decompose due to either biodegradation or hydrolysis have lower potential for emission to the air as gases.

Emission Model Input Parameters

There are various parameters that impact the estimated volatilization emission rates. In general, there are: 1) input parameters specific to the physical and chemical properties of the constituent being modeled; 2) input parameters relating to the physical and chemical characteristics of the waste material being managed; 3) input parameters specific to the process and operating conditions of the WMU being modeled; and 4) meteorological input parameters that impact both emissions and dispersion.

Table D.3-1 presents the waste and unit specific input parameters required for aerated tanks. For the deterministic modeling approach, emission estimates were developed for two representative wastewaters, one associated with a maximum generation rate and the other with a central tendency generation rate. The parameter values used in estimating emissions for both cases are shown in Table D.3-1. Also identified in this table are the parameters that were varied as part of the probabilistic analysis. The range of parameter values used in the probabilistic analysis are provide in Appendix K. More detailed discussion of each input parameter follows.

Chemical-Specific Input Parameters

Key chemical-specific input parameters include: air-liquid equilibrium partitioning coefficient (vapor pressure or Henry's law constant), liquid-solid equilibrium partitioning coefficient (log octanol-water partition coefficient for organics), biodegradation rate constants, and liquid and air diffusivities. A number of these chemical specific properties are provided in Appendix C. Those chemical specific parameters that were used exclusively in the CHEMDAT8 modeling and not elsewhere in the analysis are provided in Table D.3-2. The parameters included in this table are Antoine’ coefficients (for adjusting vapor pressure to temperature), biodegradation rate constants (biorate Kmax and Monod K1), and hydrolysis rates (which are actually the photolysis rate constant plus hydrolysis rate constant).

Table D.3 -1. CHEMDAT8 Inputs for Aerated Tanks

Input ID No.	Input Parameter	Deterministic Analysis: Parameter Value Maximum Waste Tank	 Central Tendency Waste Tank	Varied for Probabilistic Analysis	Data Source
T1	Windspeed (m/s)	Site-specific (3 locations modeled)		yes	Set by location of tank
T2	Depth (m)	4.6	4.6	no	Assumed value = 4.6 m (provided by EPA).
T3	Area (m^2)	1147	384	yes	Calculated based on waste generation rate and 2 day residence time assumption.
T4	Flow rate (m^3/yr)	9.63e+05	3.22e+05	yes	Generation rates converted to volumetric flow using an assumed wastewater density of 1g/cm^3 (equal to water).
T5	Active biomass or mixed liquor volatile suspended solids (g/L)	2	2	no	Default value used in the development of chemical-specific biodegradation rates used in CHEMDAT8 (Research Triangle Institute, 1988).
T6	Biomass solids (or TSS) conc in influent (g/L)	0.349	0.349	no	Used average TSS concentration of waste stream from sampling data.
T7	VO inlet conc. (constituent conc. in influent) (mg/L)	Chemical-specific	Chemical-specific	yes	Modeling conducted using both the average and maximum conc.
T8	Total organic conc. (TOC) in influent (mg/L)	498.17	498.17	yes	Used average TOC from sampling data.
T9	Total biorate (mg/g bio-h)	19	19	no	Default value specified in CHEMDAT8. Sensitivity analysis indicates that this parameter has minimal impact on emission estimates.
T10	Fraction agitated	0.75	0.75	no	HI - Aeration rate assumed for situations where agitation is used for biological treatment. Engineering judgment.
T11	Submerged air flow (m^3/s)	0	0	no	Set equal to 0; assumed mechanical surface mixing only.
T12	Number of aerators (unitless)	2	1	yes	Engineering judgment.
T13	Oxygen trans. rating (lbO_2/h-HP)	3	3	no	Typical value applied in EPA's *Hazardous Waste TSDF Background Information for Proposed RCRA Air Emission Standards* (U.S. EPA, 1991). Model shown to be insensitive to this parameter.
T14	Power (total)(HP)	115	80	yes	Range of 80-150 hp per million gallons of tank expected for HI aeration power. Based on information from *Wastewater Engineering: Treatment Disposal and Reuse* (Metcalf and Eddy, 1979).
T15	Power efficiency	0.83	0.83	no	U.S. EPA (1991). Typical range 0.80 to 0.85.
T16	Temperature (°C)	Site-specific (3 locations modeled)		yes	Set by location of tank.
T17	Impeller diameter (cm)	61	61	no	U.S. EPA (1991 and 1994). Input used for all aerated units.
T18	Impeller speed (rad/s)	126	126	no	CHEMDAT8 default value (U.S. EPA, 1994) for aerated unit. Sensitivity analysis indicates that this parameter has little impact on emission estimates.

Table D.3-2. (continued)

Table D.3 -2. Additional Chemical-Specific Inputs

	VAPOR PRESSURE COEFFICIENTS					
WWT CONSTITUENTS	A	B	C	Biorate Kmax mgVO/g-hr.	Monod K1 L/g-hr.	HYDROL. SEC-1
ACETONE	7.12	1210.60	229.66	1.30	1.15	0
ALLYL CHLORIDE	7.58	1493.91	273.16	10.76	0.31	0
BENZOIC ACID	9.03	3333.30	273.00	17.56	0.69	0
BENZYL ALCOHOL	7.20	1632.59	172.79	17.56	0.59	0
BIS(2-CHLOROETHYL)ETHER	8.21	2404.33	273.16	10.76	0.54	0
BIS(2-CLOROISOPROPYL)ETHER	0	0	0	129.00	1.29	0
BIS(2-ETHYLHEXYL)PHTHALATE	10.84	5228.52	273.16	0.77	0.35	0
BROMODICHLOROMETHANE	7.97	1846.56	273.16	10.76	0.70	0
BROMOFORM	7.99	2158.65	273.16	10.76	1.01	0
CARBON DISULFIDE	6.94	1169.11	241.59	15.30	0.89	0
CHLORO-1,3-BUTADIENE, 2-	6.83	1163.80	226.34	10.76	0.22	0
CHLOROBENZENE	6.98	1431.05	217.55	0.39	10.00	0
CHLORODIBROMOMETHANE	8.22	2100.17	273.16	10.76	0.04	0
CHLOROFORM	6.49	929.44	196.03	28.00	0.79	0
CRESOL(-o)	7.43	1744.32	194.44	23.21	17.00	0
CRESOL(-p)	7.04	1511.08	161.85	23.21	17.00	0
DICHLOROETHANE, 1,2-	7.07	1292.54	225.00	2.10	0.98	0
DICHLOROETHYLENE 1,2 - trans	6.97	1141.90	231.90	10.76	0.49	0
DICHLOROETHYLENE, 1,2 - cis	0	0	0	10.76	0.50	0
DIETHYL PHTHALATE	0	0	0	100.00	1.20	0
DIMETHYL PHTHALATE	4.52	700.31	51.42	2.20	3.10	0
DI-n-OCTYL PHTHALATE	7.00	2621.43	146.16	15.30	0.55	0
ETHYL CHLORIDE	6.99	1030.01	238.61	10.76	0.47	0
ETHYLBENZENE	6.98	1424.26	213.21	6.80	2.10	0
HEXACHLOROBENZENE	9.55	3248.57	203.07	0.001	0.03	0
MERCURY	0	0	0	1.00	0.00	0
METHYL ETHYL KETONE	7.11	1305.01	229.27	2.00	0.20	0
METHYLENE CHLORIDE	6.97	1074.29	223.00	18.00	0.38	0
PENTACHLOROPHENOL	8.30	3161.36	273.16	130.00	3.40	0
PHENOL	7.13	1516.79	174.95	97.00	13.00	0
STYRENE	6.95	1437.43	208.38	31.10	0.11	0
TETRACHLOROETHYLENE	6.98	1386.92	217.53	6.20	0.68	0
TRICHLOROETHYLENE	6.52	1018.60	192.70	3.90	0.88	0.12
TRICHLOROPHENOL 2,4,5	8.58	2974.58	273.16	15.30	4.48	0
TRICHLOROPHENOL 2,4,6	9.70	3528.12	273.16	17.56	0.26	0
HpCDD, 1,2,3,4,6,7,8-	0	0	0	0.001	0.03	0
HpCDF, 1,2,3,4,6,7,8-	0	0	0	0.001	0.03	0
HpCDF, 1,2,3,4,7,8,9-	0	0	0	0.001	0.03	0

(continued)

Table D.3-2. (continued)

	VAPOR PRESSURE COEFFICIENTS					
				Biorate Kmax	Monod K1	HYDROL.
WWT CONSTITUENTS	A	B	C	mgVO/g-hr.	L/g-hr.	SEC-1
HxCDD, 1,2,3,4,7,8-	0	0	0	0.001	0.03	0
HxCDD, 1,2,3,6,7,8-	0	0	0	0.001	0.03	0
HxCDD, 1,2,3,7,8,9-	0	0	0	0.001	0.03	0
HxCDF, 1,2,3,4,7,8-	0	0	0	0.001	0.03	0
HxCDF, 1,2,3,6,7,8-	0	0	0	0.001	0.03	0
HxCDF, 1,2,3,7,8,9-	0	0	0	0.001	0.03	0
HxCDF, 2,3,4,6,7,8-	0	0	0	0.001	0.03	0
OCDD, 1,2,3,4,5,7,8,9-	0	0	0	0.001	0.03	0
OCDF, 1,2,3,4,6,7,8,9-	0	0	0	0.001	0.03	0
PeCDF, 2,3,4,7,8-	0	0	0	0.001	0.03	0
TCDD, 2,3,7,8-	6.98	2377.00	159.00	0.001	0.03	0
TCDF, 2,3,7,8-	0	0	0	0.001	0.03	0

The primary data source for the parameters identified on Table D.3-2 is the CHEMDAT8 chemical properties database (U.S. EPA, 1994). For those chemicals not found in this database, the Antoine's coefficients were set to zero. These parameters are used to adjust vapor pressure (reported for 25 degrees C) to temperature (the model applies the annual average temperature specified for the site being modeled). Because the annual temperature for the sites being modeled were less than 25 degrees, setting these parameters to zero (no adjustment of vapor pressure was made) resulted in slightly higher emission estimates. For those compounds reported with biodegradation rates that appeared to be unrealistic, the biodegradation rate constants in the downloaded CHEMDAT8 database file were compared with the values reported in the summary report that served as the basis for the CHEMDAT8 tank biodegradation rate values (Research Triangle Institute (RTI), 1988). For example, the biodegradation rate constants for 2,3,7,8-TCDD in the downloaded CHEMDAT8 file were deemed to be entirely unrealistic. Therefore, the biodegradation rates constants for dioxins were assigned biodegradation rate constants equal to lindane, which was the most similar compound in the original biodegradation rate database documentation report. Biodegradation rates for compounds not in the CHEMDAT8 chemical properties database, rates were obtained from RTI (1988) or rates for similar compounds in the database were applied.

The CHEMDAT8 model was developed for estimating organic emission estimates. The CHEMDAT8 model uses the log Kow to estimate adsorption (m3/ kg solids) for each chemical. As a simplifying step for modeling mercury emissions, it was assumed that the log Kow = log Koc = log Kd. Therefore, a log Kd value (4.9) was input into the CHEMDAT8 model in the column labeled "log octanol/water part" and used to estimate sorption for mercury.[1] The model

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[1] Based on data provided in the Mercury Report Congress (U.S. EPA 1997), a Kd value of 1000 is presented in Appendix C. This updated value is used in all other modeling efforts conducted as part of this assessment. However, the updated Kd value was not used in the CHEMDAT8 modeling (that is, a log Kd of 4.9 [RTI 1995] was used instead of the updated value of 3). As discussed, the model is fairly insensitive to this parameter. Consequently, the overall impact on mercury emission estimates is negligible.

is fairly insensitive to this input parameter. For example, the following emission estimates were obtained when the logKd was set equal to 6, 4.9, 3, and 1, respectively, 6.16e-4Mg/yr, 7.24e-4 Mg/yr, 7.57e-4 Mg/yr, and 7.58e-4 Mg/yr. Given the volatile nature of mercury, applying this simplifying step in the CHEMDAT8 model allows reasonable emission estimates to be developed for this compound.

Waste Specific Input Parameters

As this analysis considered only wastewater treatment, there are only a limited number of waste specific input parameters that affect the emission estimates. The most important waste specific input parameter for emissions modeling is the constituent concentrations present in the waste (Input ID No. T7). The waste stream constituent concentrations were derived from waste stream chemical analysis data.

Other waste stream specific input parameters are "biomass solids in," "total organics in," and "total biorate" (Input ID No. T6, T8, and T9). These parameters primarily impact the amount of solids available for contaminant absorption. The "biomass solids in" does not affect the biodegradation rate and is more appropriately labeled simply "solids in", and this parameter was estimated from total suspended solids (TSS) analysis of the influent waste stream. Similarly, the "total organics in" input was estimated from the total organic content (TOC) analysis of the influent waste stream. The "total biorate" is a measure of how fast the TOC is converted to new biomass, so that it can be considered a measure of the overall biodegradability of the TOC in the wastewater influent. The CHEMDAT8 default value was used for this parameter. These "other" waste stream parameters typically have little impact on the predicted emission rate, but as the primary removal mechanism for dioxins in aerated tanks tends to be adsorption, these inputs have a potential to impact the calculated emission rates.

WMU Specific Input Parameters

The annual waste quantity (flow rate) and the dimensions of the tank are critical input parameters for wastewater tanks. Site specific / unit specific data were not available for the aerated tanks; therefore, the flow rate and dimensions of the tanks were estimated based on reported annual waste quantities, an assumed retention time of 2 days, and an assumed tank depth of 4.6 m.

Factors that impact the relative surface area of turbulence and the intensity of that turbulence are important factors in determining the fate of chemicals in aerated tanks. The aerated tank model has several input parameters that impact the degree and intensity of the turbulence created by the aeration (or mixing). These inputs parameters include Input ID No. T10, T11, T12, T13, T14, T15, T17 and T18 (see Table D.3-1).

Factors that influence the rate of biodegradation are important in determining emissions from aerated tanks. The active biomass concentration (Input ID No. T5) is a critical parameter for aerated tanks. CHEMDAT8 aerated tank default value of 2.0 g/L was used for the biomass concentration because this is reasonable, but low-end value, for biomass concentrations present in activated sludge wastewater treatment tanks.

Meteorological Specific Input Parameters

Meteorological inputs are also important for the aerated tank emission model. The emission estimates are impacted by both temperature and wind speed (Input ID No. T1 and T16). The annual average temperature and wind speed for the given meteorological location were used in the analysis.

Model Sensitivity

A sensitivity analysis was performed on the CHEMDAT8 aerated unit emission model to investigate the impact that the input parameters specified in Table D.3-1 have on overall emission estimates. As part of this analysis, the emission estimates obtained for Baton Rouge using the central tendency waste tank size and average constituent concentrations were used as the baseline emissions. The analysis was performed by varying a single parameter one at time. The goal of the exercise was to estimate the impact that a single input parameter had on the overall emission estimates. In most cases, the input parameters were varied by a factor of two. The only parameters that were not varied by a factor of 2 included the aerator power efficiency and fraction agitated; an efficiency of 0.5 was used (rather than 0.83 ÷ 2; a typical variation for this parameter is from 0.80 to 0.85) and fraction agitated was set equal to 1 (rather than 0.75 x 2). Results from this analysis are summarized in Table D.3-3. As seen from this table, the aerated tank model is most sensitive to the constituent concentration and the waste flow rate. Other parameters that impact emissions to a lesser extent include active biomass, fraction agitated, total power, and depth. The parameters that had little impact on overall average emissions (i.e., less 20% increase or decrease) were TOC in influent, TSS in influent, total biorate, number of aerators, oxygen transfer rate, power efficiency, and impeller diameter and speed.

Development of Volatile Emissions and Waste Concentrations for Tanks

The basic modeling assumptions used (or inherent in CHEMDAT8) for the aerated tank model emission estimates include:

- The tank operates at steady state.
- The tank is well-mixed.
- The waste matrix is aqueous (Henry's law partitioning applies).
- Temperature determined by assigned meteorological stations; used annual average temperatures.
- Biodegradation rate is first order with respect to biomass concentrations.
- Biodegradation rate follows Monod kinetics with respect to contaminant concentrations.
- Hydrolysis rate is first order with respect to contaminant concentrations.

Table D.3-3. Sensitivity Analysis for CHEMDAT8 Aerated Tank Emissions

CHEMDAT8 Input Parameter	Overall Average Increase or Decrease in Emissions From Baseline Emission Estimates	
	When Base Parameter Value (Table D.3-1) was Increased by Factor of 2[a]	When Parameter Value (Table D.3-1) was Decreased by Factor of 2[a]
Depth (meters)	24% decrease	37% increase
Surface area (m^2)	24% increase	12% decrease
Flow (m^3/yr)	65% increase	34% decrease
Active Biomass or mixed liquor volatile suspended solids (g/L)	23% decrease	35% increase [b]
Total suspended solids (TSS) concentration in influent (g/L)	12% decrease	13% increase
Constituent concentration in influent (mg/L)	Factor of 2 increase	50% decrease
Total organic concentration in influent (mg/L)	10% decrease	9% increase
Total biorate (mg/g bio-hr)	0.2% increase	0.2% increase
Fraction agitated (unitless)	21% increase (Frac. agitated set equal to 1)	33% decrease
Number of Aerators (unitless)	16% decrease (No. Aerators set equal to 2)	NA
Oxygen transfer rate (lb O_2/h-hp)	6% increase	7% decrease
Total power (hp)	27% increase	22% decrease
Power efficiency (unitless)	NA	5% decrease (set equal to 0.50)
Impeller diameter (cm)	15% decrease	19% increase
Impeller speed (rad/s)	8% decrease	10% increase

[a] Unless otherwise noted.

[b] When Active Biomass or mixed liquor volatile suspended solids (g/L) was set equal to zero, overall average emissions increased by a factor of 80.

For tanks, the surface area, depth, and flow rate are all directly specified by the model units. As part of the deterministic modeling, two model units were run: an average size tank and a large tank, based on the reported annual waste volumes. The emissions from these units were modeled at the selected meteorological regions. As part of the Monte Carlo modeling effort, depth was held constant but surface area and flow rate were varied.

CHEMDAT8 tank model calculates the mass fraction of influent contaminant that is emitted, biodegraded, adsorbed, or hydrolyzed. Based on the fraction emitted, the model calculates an annual emission rate. The only output required from CHEMDAT8 for the risk analysis is the air emissions rate in units of g/m^2-s. The desired emission rate, in g/m^2-s, can be calculated either from the CHEMDAT8 estimated emission rate (megagrams/year), the unit's surface area, and appropriate unit conversion factors as shown in Equation D.3 -3 or from the CHEMDAT8 estimated fraction emitted, the flow rate (Q_{flow}), constituent-specific waste concentration in the influent (C_{infl}), and the unit's surface area as shown in Equation D.3-4:

$$Emiss.Rate\ (g/m2-s) = \frac{Emiss.Rate\ (Mg/year)\ x\ 3.2e-08\ (yr/s)\ x\ 1e+06\ (g/Mg)}{Area(m^2)} \tag{3}$$

$$Emiss.Rate\ (g/m2-s) = \frac{Q_{flow}(m^3/s)\ x\ C_{infl}(g/m^3)\ x\ Emiss.Fract.}{Area(m^2)} \tag{4}$$

ISCST3 Model for Air Dispersion and Deposition

Results of air dispersion and deposition modeling represent the initial fate and transport of vapor and particle emissions in the environment. Air dispersion modeling was conducted with EPA's Industrial Source Complex Short Term, version 3 (ISCST3 - dated 12/23/98). The ISCST3 model and meteorological preprocessor, PCRAMMET, and related user's guides can be accessed and downloaded through the Internet from the Support Center for Regulatory Air Models (SCRAM) web page (http://www.epa.gov/scram001). The SCRAM is part of the EPA OAQPS Technology Transfer Network (TTN).

Modeling was conducted to estimate the dispersion and deposition of vapors emitted from the chlorinated aliphatics wastewater treatment tank, the EDC/VCM sludge municipal landfill, the methyl chloride sludge onsite industrial landfill, and the EDC/VCM sludge land treatment unit. EPA also used ISCST3 to estimate the dispersion and deposition of particulate emissions from the land treatment unit. ISCST3 was used to estimate:

- the air concentration of vapors,
- wet deposition of vapors onto soils and surface water,
- the air concentration of particulates,
- wet deposition of particles onto soils and surface water, and
- dry deposition of particles onto soils, surface water, and plants.

We estimated dry deposition of vapors onto soils using a dry deposition algorithm for particles (from the ISCST user's manual) with an assumed deposition velocity of 0.2 centimeters per second (cm/s) (Koester and Hites, 1992). This approach tends to overestimate dry deposition for lipophilic compounds because a significant fraction, approximately 25 to 75 percent, is typically bound to particles (Trapp and Matthies, 1998). Nevertheless, this approach has been used by EPA in other analyses that evaluate risks from exposure to dioxin, such as the hazardous waste combustion risk assessment. The approach assumes that dioxin vapors behave as fine aerosols and, therefore, are amenable to modeling using the dry deposition algorithm for particles.[2] EPA decided that this was a reasonable alternative to use for all organic constituents until the dry deposition algorithm becomes available in the ISC model.

In the absence of onsite meteorological data, modeling was conducted using data obtained from representative meteorological locations. For the EDC/VCM sludge municipal landfill, modeling was conducted for the 50th percentile of the municipal landfill area distribution (60,705 m^2) using meteorological data obtained from Baton Rouge, LA, and Houston, TX, meteorological stations. Based on rainfall, infiltration, runoff, and erosion values, we selected Baton Rouge and Houston to represent high end and central tendency locations, respectively. Modeling of the methyl chloride sludge onsite industrial landfill (83,610 m^2)was conducted using meteorological data from Louisville, KY, to represent the Carrollton, KY, site. Baton Rouge data (the representative meteorological station for the Plaquemine, LA site) were used to model the 687,990 m^2 EDC/VCM sludge LTU.

Chlorinated aliphatic wastewaters were evaluated with both a deterministic and probabilistic modeling approach. For the deterministic analysis, modeling was conducted for both the maximum and central tendency sized waste tanks. For the probabilistic analysis, modeling was conducted for eight tank sizes (surface area was varied but height was held constant). These tanks were selected to represent the range of possible wastewater treatment tanks. Under both analyses, it was assumed that the tanks were partially above ground and partially below ground. The height of the tank was specified as 10 ft (the depth of the water in the tank was set at 15 ft; the height of the tank above ground is half of the depth of water plus 2.5 ft of freeboard).

As part of the initial ISCST3 modeling effort, which was designed to select representative high-end and central tendency meteorological stations, modeling was conducted for the maximum and central tendency sized tanks. Receptor points were placed in 16 directions at distances of 75 and 300 m from the edge of the units. Modeling was conducted using meteorological data obtained from a set of 11 meteorological stations. These stations were selected to be representative of the climatic regions associated with each of the 23 facilities of interest. The facility location associated with each of the representative meteorological stations is shown in Section 2, Table 2-5.

An analysis of the air dispersion modeling results was conducted to identify meteorological locations that would serve as the central tendency and high end locations for the risk assessment. In conducting this analysis, both the air concentration and wet deposition of vapor rates were considered. For each type of dispersion output, four sets of data were reviewed. These data sets correspond to each of the tank size (central tendency waste tank and high end waste tanks)/ receptor distance (75 and 300 m) combinations modeled. These data are shown in Table D.3-4. Based on an analysis on the data shown, three meteorological locations were identified for inclusion in the assessment:

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[2] Koester and Hites (1992) suggest that the dry deposition of vapor may be negligible.

Table D.3-4. ISCST3 Air Dispersion Model Results and Analysis

Station Name	Tank Size	Receptor Distance (m)	Station Number	Temp. (deg. F)	Wind Speed (m/s)	Max Air Conc (ug/m^3) / (mg/s-m^2)	Max Wet Dep (g/m^2/yr) / (mg/s-m^2)
New Orleans, LA	Central	75	12916	69	4.12	33.29	0.242
Baton Rouge, LA	Central	75	13970	68	4.12	51.65	0.301
Lake Charles, LA	Central	75	3937	68	4.63	45.33	0.208
Memphis, TN	Central	75	13893	65	3.60	54.76	0.225
Houston, TX	Central	75	12960	69	4.12	43.34	0.186
Louisville, KY	Central	75	93821	57	4.12	59.19	0.212
Baltimore, MD	Central	75	93721	56	4.63	66.99	0.224
Evansville, IN	Central	75	93817	53	4.63	46.63	0.233
Albany, NY	Central	75	14735	48	5.14	60.70	0.311
Flint, MI	Central	75	14826	47	5.14	50.91	0.207
Wichita, KS	Central	75	3928	57	6.17	72.70	0.128
New Orleans, LA	Central	300	12916	69	4.12	4.79	0.063
Baton Rouge, LA	Central	300	13970	68	4.12	8.38	0.080
Lake Charles, LA	Central	300	3937	68	4.63	7.14	0.057
Memphis, TN	Central	300	13893	65	3.60	8.59	0.063
Houston, TX	Central	300	12960	69	4.12	6.63	0.050
Louisville, KY	Central	300	93821	57	4.12	9.52	0.055
Baltimore, MD	Central	300	93721	56	4.63	11.97	0.056
Evansville, IN	Central	300	93817	53	4.63	6.69	0.060
Albany, NY	Central	300	14735	48	5.14	8.81	0.087
Flint, MI	Central	300	14826	47	5.14	7.98	0.058
Wichita, KS	Central	300	3928	57	6.17	11.47	0.037
New Orleans, LA	Maximum	75	12916	69	4.12	88.54	0.663
Baton Rouge, LA	Maximum	75	13970	68	4.12	132.85	0.829
Lake Charles, LA	Maximum	75	3937	68	4.63	116.80	0.547
Memphis, TN	Maximum	75	13893	65	3.60	145.80	0.588
Houston, TX	Maximum	75	12960	69	4.12	112.60	0.489
Louisville, KY	Maximum	75	93821	57	4.12	161.31	0.583
Baltimore, MD	Maximum	75	93721	56	4.63	176.90	0.632
Evansville, IN	Maximum	75	93817	53	4.63	121.32	0.637
Albany, NY	Maximum	75	14735	48	5.14	158.23	0.813
Flint, MI	Maximum	75	14826	47	5.14	132.87	0.535
Wichita, KS	Maximum	75	3928	57	6.17	178.40	0.322
New Orleans, LA	Maximum	300	12916	69	4.12	13.74	0.183
Baton Rouge, LA	Maximum	300	13970	68	4.12	23.84	0.231
Lake Charles, LA	Maximum	300	3937	68	4.63	20.29	0.163
Memphis, TN	Maximum	300	13893	65	3.60	24.60	0.181
Houston, TX	Maximum	300	12960	69	4.12	18.92	0.145
Louisville, KY	Maximum	300	93821	57	4.12	27.28	0.161
Baltimore, MD	Maximum	300	93721	56	4.63	33.91	0.164
Evansville, IN	Maximum	300	93817	53	4.63	19.15	0.175
Albany, NY	Maximum	300	14735	48	5.14	25.30	0.253
Flint, MI	Maximum	300	14826	47	5.14	22.77	0.168
Wichita, KS	Maximum	300	3928	57	6.17	32.50	0.106

(continued)

Table D.3-4. (continued)

Central& 75 m	Maximum Air Concentration of Vapor				Maximum Wet Dep of Vapor			
	Point	*Column1*	*Rank*	*Percent*	*Point*	*Column1*	*Rank*	*Percent*
	11	72.696	1	100.00%	9	0.31093	1	100.00%
	7	**66.993**	**2**	**90.00%**	**2**	**0.3011**	**2**	**90.00%**
	9	60.696	3	80.00%	1	0.242	3	80.00%
	6	59.186	4	70.00%	8	0.23259	4	70.00%
	4	**54.757**	**5**	**60.00%**	**4**	**0.22471**	**5**	**60.00%**
	2	51.647	6	50.00%	7	0.22389	6	50.00%
	10	50.9097	7	40.00%	6	0.21165	7	40.00%
	8	46.63121	8	30.00%	3	0.208	8	30.00%
	3	45.33	9	20.00%	10	0.20722	9	20.00%
	5	43.34	10	10.00%	5	0.186	10	10.00%
	1	33.29	11	.00%	11	0.1276	11	.00%

Cent. Tank & 300 m	Maximum Air Concentration of Vapor				Maximum Wet Dep of Vapor			
	Point	*Column1*	*Rank*	*Percent*	*Point*	*Column1*	*Rank*	*Percent*
	7	**11.965**	**1**	**100.00%**	9	0.08703	1	100.00%
	11	11.472	2	90.00%	**2**	**0.08**	**2**	**90.00%**
	6	9.524	3	80.00%	1	0.0629	3	80.00%
	9	8.807	4	70.00%	**4**	**0.0625**	**4**	**70.00%**
	4	**8.5883**	**5**	**60.00%**	8	0.05986	5	60.00%
	2	8.3805	6	50.00%	10	0.05829	6	50.00%
	10	7.97856	7	40.00%	3	0.0565	7	40.00%
	3	7.138	8	30.00%	7	0.05593	8	30.00%
	8	6.69016	9	20.00%	6	0.05523	9	20.00%
	5	6.63	10	10.00%	5	0.05	10	10.00%
	1	4.79	11	.00%	11	0.03684	11	.00%

Max Tank & 75 m	Maximum Air Concentration of Vapor				Maximum Wet Dep of Vapor			
	Point	*Column1*	*Rank*	*Percent*	*Point*	*Column1*	*Rank*	*Percent*
	11	178.4	1	100.00%	**2**	**0.82852**	**1**	**100.00%**
	7	**176.899**	**2**	**90.00%**	9	0.81316	2	90.00%
	6	161.31	3	80.00%	1	0.663	3	80.00%
	9	158.232	4	70.00%	8	0.637	4	70.00%
	4	**145.8**	**5**	**60.00%**	7	0.632	5	60.00%
	10	132.87	6	50.00%	**4**	**0.588**	**6**	**50.00%**
	2	132.846	7	40.00%	6	0.5826	7	40.00%
	8	121.324	8	30.00%	3	0.547	8	30.00%
	3	116.8	9	20.00%	10	0.5347	9	20.00%
	5	112.6	10	10.00%	5	0.489	10	10.00%
	1	88.54	11	.00%	11	0.322	11	.00%

Max Tank & 300 m	Maximum Air Concentration of Vapor				Maximum Wet Dep of Vapor			
	Point	*Column1*	*Rank*	*Percent*	*Point*	*Column1*	*Rank*	*Percent*
	7	**33.914**	**1**	**100.00%**	9	0.25259	1	100.00%
	11	32.5	2	90.00%	**2**	**0.23142**	**2**	**90.00%**
	6	27.282	3	80.00%	1	0.183	3	80.00%
	9	25.304	4	70.00%	**4**	**0.181**	**4**	**70.00%**
	4	**24.6**	**5**	**60.00%**	8	0.17484	5	60.00%
	2	23.836	6	50.00%	10	0.1682	6	50.00%
	10	22.77	7	40.00%	7	0.164	7	40.00%
	3	20.29	8	30.00%	3	0.163	8	30.00%
	8	19.147	9	20.00%	6	0.16141	9	20.00%
	5	18.92	10	10.00%	5	0.145	10	10.00%
	1	13.74	11	.00%	11	0.106	11	.00%

Baltimore to represent the **high end** site for air concentration
Baton Rouge to represent the **high end** site for wet deposition of vapor
Memphis to represent the **central tendency** site for both air concentration and wet deposition of vapor.

Ideally, only two locations would have been selected, one for central tendency and one for high-end modeling. The reason that two high-end sites were identified is because there was no single site that had high-end results for both air concentration and wet deposition of vapor. Given that the waste being modeled is assumed to contain quite a range of chemicals, it was recommended that the two different high-end sites be included. By including the extra location, the likelihood of underestimating inhalation risks (driven by air concentration) or indirect risks (driven by air concentration and/or deposition, depending on the constituent) will be minimized.

Once the representative meteorological locations were selected, additional modeling for the sites was conducted for use in the deterministic and probabilistic analysis.

Preparing ISCST3 Input Files

Two input files are required to run ISCST3, the control file and the meteorological file. The control file (*.inp) is an ASCII file that contains the model option settings, source parameters, and receptor locations. The meteorological file (*.met) contains hourly values for a number of parameters including wind speed, wind direction, stability class, mixing height, ambient air temperature, and precipitation type and amount.

Control File

ISCST3 requires inputs for source parameters, receptor locations, meteorological data, and, in some cases, terrain features. These data are input to the model through the use of a control file. The control file is divided into the sections or pathways shown in Table D.3-5. Each pathway is identified in the control file by two letters. Keywords associated with each pathway are specified by the user to control the model run and define site specific modeling conditions. Each of the control file pathways and how they were specified for this analysis are described below. The ISC3 User's Guide (U.S. EPA, 1995b) provides detailed guidance for preparing control files.

Control Pathway

Under the control pathway, the user specifies keywords that determine whether the model will calculate air concentrations or deposition rates. In addition, modeling options that are to be applied as part of these calculations are specified. Keywords used in the control pathway include MODELOPT (controls modeling options), AVERTIME (identifies averaging period to be calculated for the run - annual for this analysis), and POLLUTID (identifies the type of pollutant being modeled).

The user specifies the type of model output desired through the use of secondary keywords. For this analysis, the outputs desired for vapor phase included air concentration (CONC) and wet deposition (WDEP), and the desired outputs for particle phase modeling

Table D.3-5. ISCST3 Control File Pathways

Pathways	Identifier	Use
Control Options	CO	Provides overall control of the model run (e.g., modeling options are selected)
Source Characteristics	SO	Defines emission source information for the model run
Receptor Locations	RE	Defines receptor information for the model run
Meteorological Data	ME	Defines the meteorological data for the model run
Terrain File	TG	Defines the input terrain information for the model run (not applicable for area sources such as LTUs)
Output Options	OU	Defines output options for the model run

included air concentration (CONC), wet deposition (WDEP), and dry deposition (DDEP).[3] Combined deposition rates are also required as input to the indirect exposure modeling process but they were not calculated by the ISCST3. Alternatively, these rates were estimated by externally summing the wet and dry deposition rates.

ISCST3 is a Gaussian plume model that can simulate plume depletion. In calculating outputs for both vapors and particles, the wet plume depletion option was activated through the use of the secondary keyword WETDPLT. With the current version of ISCST3, dry plume depletion cannot be calculated for vapors, and, for particles, the run times associated with dry plume depletion were excessive. Preliminary model runs for particles indicated that use of the dry plume depletion option significantly increased run times for a large area source (approximately 2 weeks compared to 1 day). Review of data obtained for runs conducted with depletion and those without depletion activated indicated that air concentrations and dry deposition rates, respectively, are higher when dry plume depletion is not calculated.

Another modeling option that is controlled by the MODELOPT keyword is whether the model is run in rural or urban mode. This distinction is based on the land use within a 3-km radius from the emission source. These modes differ with respect to dispersion parameters, wind profile exponent, and temperature gradients. Unless the site is located in a heavily metropolitan area, the rural option is generally more appropriate. Because the types of waste management units being assessed are typically in nonurban areas, the rural option was used in this analysis.

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[3] Dry deposition of vapors is needed as input to the indirect modeling but this output cannot be calculated using the current version of ISCST3 (dated 12/28/98). Dry deposition of vapors was calculated as the product of vapor air concentration times an assumed dry deposition velocity (0.2 cm/s).

Source Characteristics Pathway

Under the source pathway, the user provides information to characterize the emission source being modeled. Two mandatory source pathway keywords are LOCATION and SRCPARAM.

The information provided following the LOCATION keyword identifies the source type and location. For this analysis, the source types specified included elevated (tanks) and ground based (LTU and landfills) square-shaped area sources. For an area source, location is identified by specifying the x- and y- coordinates of the southwest corner of the source. In the absence of site specific information, a square source with sides parallel to X- and Y- axes was modeled. The x- and y-coordinates of the southwest corner of the source were specified according to the size of the waste management unit. The EDC/VCM LTU size was about 688,000 m^2 or about 829 m × 829 m. The approximate sizes of the landfills modeled were 246 m × 246 m for the EDC/VCM sludge municipal landfill and 289 m x 289 m for the methyl chloride sludge onsite industrial landfill. The two tanks sizes modeled as part of the deterministic analyses were 1147 m^2 (approximately 34 m x 34 m) and 384 m^2 (approximately 20 m x 20 m). Modeling for the probabilistic analysis for tanks included eight sized tanks: 10.8 m x 10.8 m; 12.3 m x 12.3 m; 13.7 m x 13.7 m 14.4 m x 14.4 m; 19.4 m x 19.4 m; 19.6 m x 19.6 m; 22.3 m x 22.3 m; and 33.9 m x 33.9.

The SCRPARAM keyword is used to provide information on source parameters such as emission rate and source dimensions. For this analysis, the ISCST3 air model was run using a unit emission rate of 1 $\mu g/m^2$-s. Adjustments for chemical-specific emission rates occur later in the indirect modeling process as discussed below. The source-specific dimensions required as input for an area source include

- Release height above ground in meters (set equal to 0 for the LTU and landfills and to 10 feet or 3.05 meters for the tanks)
- Length of x- side of the area in meters
- Length of y- side of the area in meters
- Orientation angle (set equal to 0)
- Initial vertical dimensions of the plume (set equal to release height/2.15).

Following the SCRPARAM keyword line, particle size distributions, particle diameter, particle density, and scavenging coefficients are input to the particle control file while gas scavenging coefficients are input to the vapor control file. Table D.3-6 identifies the particle size

Table D.3-6. Particle Size Distribution and Scavenging Coefficients

Particle Size Diameter (µm)	Weight Distribution (Fraction)	Liquid and Frozen Scavenging Coefficients (h/mm-s)
5.0	0.50	3.7E-4
20.0	0.50	6.7E-4

distribution and the associated scavenging coefficients that were applied for particles. The scavenging coefficients associated with the particle size distribution shown were obtained from Jindal and Heinhold (1991). Liquid and frozen scavenging coefficients were set equal (PEI, 1986). A vapor scavenging coefficient of 1.7E-4 (h/mm-s) was assumed and input to the vapor control file. Although wet scavenging of vapors depends on the properties of the chemicals involved, not enough data are available to develop chemical-specific scavenging coefficients adequately at this time. Therefore, gases were assumed to be scavenged at the rate of small particles whose behavior in the atmosphere is assumed to be influenced more by the molecular processes that affect gases than the physical processes that often dominate behavior of larger particles. The value 1.7E-4 (h/mm-s) for the gas scavenging coefficient was also taken from Jindal and Heinhold (1991).

Receptor Pathway

The receptor pathway contains keywords that allow the user to specify receptor locations. For both the deterministic and probabilistic analyses, the receptor points were modeled at sixty-four and thirty-two directions, respectively, for tanks and land-based units (land treatment unit and landfills). For the deterministic analysis, receptors were specified at distances of 75 m and 300 m from the edge of the waste management units modeled. The distance of 250 ft (approximately 75 m) is based on the actual measured distance to the nearest resident for the worst-case facility evaluated in the risk assessment conducted to support the “Hazardous Waste Treatment, Storage, and Disposal Facilities - Organic Air Emissions Standards for Process Vents and Equipment Leaks Final Rule” (55 FR 25454), and was used as distance to the nearest resident for that rulemaking. In the same risk assessment, EPA identified the receptor distance of 1000 ft (approximately 300 m) as the median distance in a random sample of distances to the nearest residence. For the probabilistic analysis, we assumed the receptors live either 50, 75, 100, 200, 300, 500, or 1000 m from the waste management unit. We always assume that the receptors live in the direction associated with the highest air releases from the waste management units. Therefore, maximum concentrations and deposition rates obtained for each distance were used as input to the indirect modeling process.

Meteorological Pathway

The meteorological pathway provides information about the meteorological input data including file name, anemometer height, meteorological station identification numbers, and identification of the initial year of data in the data set.

Under this assessment, modeling was conducted using data obtained from the representative meteorological stations. To characterize long-term impacts, 5 years of meteorological data were needed as input from each of the meteorological stations. Sufficient data were available for all meteorological locations.

Control files were set up for each of the meteorological stations. The keywords included in the ME pathway of these files were INPUTFIL, ANEMHGHT, SURFDATA, and UAIRDATA. The INPUTFIL keyword is used to identify the name of the meteorological input file (*.MET). The meteorological input files created were given names that corresponded to each station’s identification number. Anemometer heights (ANEMHGHT) for each station were obtained from the Local Climatological Data, Annual Summaries (NOAA, 1982). For each location modeled, the meteorological input file combines surface observation data (SURFDATA) and twice daily mixing heights (UAIRDATA). The keywords SURFDATA and UAIRDATA in the ME pathway are followed by a station identification number and year indicating the initial year in the data set. This information is used to verify that the correct data are contained in the meteorological input file.

Terrain Pathway

The terrain pathway is used to define the terrain input file used in calculating dry depletion in elevated or complex terrain. This pathway is optional for the ISC models and was omitted from this analysis because flat terrain must be used with area sources.

Output Pathway

ISCST3 results can be generated in several different formats. For example, a table of maximum values or a table of values for each receptor can be generated. For this analysis, plotter output files were specified to facilitate averaging across field receptors. The plotter files list the x- and y-coordinates of all the modeled receptors and their corresponding air concentrations and deposition rates.

Meteorological File

The meteorological file (*.MET) is generated using the meteorological preprocessor PCRAMMET. This preprocessor pairs hourly surface observations with mixing height data. The preprocessor creates a file that contains hourly wind speed, wind direction, atmospheric stability class, temperature, and mixing height.

For each location modeled, 5 years of surface and upper air data were obtained to determine long-term annual average air concentration and deposition estimates. Surface data were obtained from the Solar and Meteorological Surface Observation Network (SAMSON) CD-ROM (NOAA, 1993). These data include 5 years of hourly observations of the following meteorologic parameters: opaque cloud cover, temperature, wind direction, windspeed, ceiling height, current weather, station pressure, and precipitation type and amount. The corresponding upper air data (i.e., twice daily mixing height data) were obtained from EPA's SCRAM (http://www.epa.gov/scram001).

In processing the meteorological data, PCRAMMET requires additional inputs for the modeled site and meteorological station. These input parameters include Anthropogenic Heat Flux, Bowen Ratio, Minimum Monin-Obukhov Length, Noontime Albedo, Fraction of Net Radiation Absorbed by the Ground, and Surface Roughness Length. In the absence of field-specific information, conditions at the modeled sited were assumed to be similar to those at the meteorological station. Therefore, the inputs for the site were set equal to those developed for the meteorological station. The inputs were developed for each meteorological location from average annual values assuming agricultural land use. Anemometer heights were obtained from the Local Climatological Data, Annual Summaries (NOAA, 1982).

Estimating Chemical-Specific Air Concentrations and Deposition Rates

To reflect the vapor-particle split of emissions, air dispersion modeling was performed separately for vapor-phase and particle-bound phase. The ISCST3 outputs obtained for vapors included air concentration and wet deposition. In a separate spreadsheet, dry deposition of vapors was calculated from the air concentration of vapors and an assumed deposition rate for vapors (0.2 cm/s). Outputs obtained for particles included: (1) wet deposition of particle, (2) dry deposition of particles, and (3) air concentration of particles. The combined deposition rate of particles was estimated by summing the results obtained for the dry and wet deposition of particles.

Modeling of each phase was conducted using a unit emission rate of 1 µg/m^2-s to obtain unitized air concentrations and deposition rates. The unitized air modeling results were converted to chemical-specific air concentrations and deposition rates for the exposure analysis. This conversion, shown below, accounts for chemical-specific emission rates (Q) and the partitioning of chemicals between the vapor and particle phases.

Vapor Phase:
All vapor phase air model outputs (i.e., air concentration and wet deposition) are multiplied by the emission rate (Q) as follows:

$$\text{Vapor phase air conc.} = \frac{\text{Unitized Air Conc. of Vapor x Chemical Specific Emission}}{\text{Unit Emission Rate}} \qquad \text{(D.3-5)}$$

$$\text{Vapor phase wet deposition} = \frac{\text{Unitized Wet Dep. of Vapor x Chemical Specific Emission}}{\text{Unit Emission Rate}} \qquad \text{(D.3-6)}$$

Particle Phase:
Similarly, all particle-bound air model outputs are multiplied by the emission rate Q.

$$\text{Particle phase air conc.} = \frac{\text{Unitized Air Conc. of Particles x Chemical Specific Emission}}{\text{Unit Emission Rate}} \qquad \text{(D.3-7)}$$

$$\text{Particle phase wet deposition} = \frac{\text{Unitized Wet Dep. of Particles x Chemical Specific Emission}}{\text{Unit Emission Rate}} \qquad \text{(D.3-8)}$$

$$Particle\ phase\ dry\ deposition = \frac{Unitized\ Dry\ Dep.\ of\ Particles\ x\ Chemical\ Specific\ Emission}{Unit\ Emission\ Rate} \qquad (D.3\text{-}9)$$

For each compound, the particle phase combined deposition was estimated by summing the chemical-specific particle phase wet deposition and particle phase dry deposition values.

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Appendix D.4

Groundwater Contaminant Fate and Transport Modeling Using EPACMTP

Appendix D.4

Groundwater Contaminant Fate and Transport Modeling Using EPACMTP

Background Information on EPACMTP

EPACMTP (EPA's Composite Model for Leachate Migration with Transformation Products) (U.S. EPA, 1996a, 1996b, 1996c, and 1997a) is a computer simulation model for modeling the subsurface fate and transport of contaminants leaching from a land disposal site, e.g., landfill, surface impoundment, wastepile, or land application unit. Fate and transport processes accounted for in the model are: advection, hydrodynamic dispersion, equilibrium linear or nonlinear sorption, and chemical and biological decay processes. The composite model consists of two coupled modules: (1) a one-dimensional module that simulates infiltration and dissolved contaminant transport through the unsaturated zone, and (2) a saturated zone flow and transport module that can be run in either 3-D or quasi 3-D mode. EPACMTP also has the capability to perform Monte Carlo simulations to account for parametric uncertainty or variability. The flow and transport simulation modules of EPACMTP are linked to a Monte Carlo driver, which permits a probabilistic evaluation of uncertainty in model input parameters, as described by specified (joint) probability distributions.

EPACMTP has been published in an international refereed journal (Kool et al., 1994) and has been reviewed by EPA's Science Advisory Board (U.S. EPA, 1995). This review commends the Agency for its significant improvements to the model and states that EPACMTP represents the state of the art for nationwide regulatory analyses (U.S. EPA, 1995).

Methods and Assumptions Used to Model Flow and Transport

EPACMTP simulates steady-state flow in both the unsaturated zone and the saturated zone; contaminant transport can be either steady state or transient. The steady-state modeling option is used for continuous source modeling scenarios; the transient modeling option is used for finite source modeling scenarios. The output of EPACMTP is a prediction of the contaminant concentration arriving at a downgradient groundwater receptor well. This can be either a steady-state concentration value, corresponding to the continuous source scenario, or a time-dependent concentration, corresponding to the finite source scenario. In the latter case, the model can calculate either the peak concentration arriving at the well, or a time averaged concentration, corresponding to a specified exposure duration, e.g., a 9-year average residence time.

Flow in the Unsaturated Zone. Flow in the unsaturated zone is assumed to be steady-state, one-dimensional vertical flow from beneath the source toward the water table. The lower boundary of the unsaturated zone is assumed to be the water table. Actual flow in the unsaturated zone is predominantly gravity-driven. Therefore, it is reasonable to model flow in the unsaturated zone as one-dimensional in the vertical direction. It is also assumed that transverse dispersion (both mechanical dispersion and molecular diffusion) is negligible in the vadose zone. This assumption is based on the fact that lateral migration due to transverse dispersion is negligibly small compared with the horizontal dimensions of waste management units. In addition, this assumption is conservative because it allows the leading front of chemicals to arrive at the water table relatively sooner and, in the case of finite source, with greater peak concentration. The flow rate is assumed to be determined by the long-term average infiltration rate through the waste management unit (WMU). In surface impoundments, the flow rate is assumed to be determined by the average depth of ponding in the impoundment, and the hydraulic conductivity and thickness of a sediment layer (or liner) at the base of the impoundment.

Transport in the Unsaturated Zone. Contaminant transport in the unsaturated zone is assumed to occur by advection and dispersion. The unsaturated zone is assumed to be initially contaminant-free, and contaminants are assumed to migrate vertically downward from the disposal facility. EPACMTP can simulate both steady-state and transient transport in the unsaturated zone with single-species or multiple-species chain decay reactions and with linear or nonlinear sorption.

Flow in the Saturated Zone. The saturated zone module of EPACMTP is designed to simulate flow in an unconfined aquifer with constant saturated thickness. The model assumes regional flow in a horizontal direction with vertical disturbance resulting from recharge and infiltration from the overlying unsaturated zone and waste disposal facility, respectively. The lower boundary of the aquifer is assumed to be impermeable. Flow in the saturated zone is assumed to be steady-state. EPACMTP accounts for different recharge rates beneath and outside the source area. Ground water mounding beneath the source is represented in the flow system by increased head values at the top of the aquifer. This approach is reasonable as long as the height of the mound is small relative to the thickness of the saturated zone.

Transport in the Saturated Zone. Contaminant transport in the saturated zone is assumed to be the result of advection and dispersion. The aquifer is assumed to be initially contaminant-free, and contaminants are assumed to enter the aquifer only from the unsaturated zone immediately underneath the waste disposal facility, which is modeled as a rectangular, horizontal plane source. EPACMTP can simulate both steady-state and transient three-dimensional transport in the aquifer. For steady-state transport, the contaminant mass flux entering at the water table must be constant with time; for the transient case, the flux at the water table may be constant or may vary as a function of time.

Treatment of Chemical-Specific First-Order Decay and Sorption

EPACMTP can simulate the transport of single-species or multiple-species chain decay reactions and also accounts for chemical and biological transformation processes. All transformation reactions are represented by first-order decay processes. These transformation processes can be lumped together and specified as an overall decay rate or specified with separate first-order decay coefficients for chemical decay and biodegradation. EPACMTP also has the capability to determine the overall decay rate from chemical-specific hydrolysis constants using soil and aquifer temperature and pH values. In the event that the daughter products of transformation are hazardous and their chemical-specific parameters are known, the model can also account for the formation and subsequent fate and transport of these daughter products.

The groundwater pathway analysis accounts for equilibrium sorption of waste constituents by the soil and aquifer solid phase. For organic constituents, a partition coefficient (K_d) is calculated as the product of the constituent-specific organic carbon partition coefficient (K_{oc}) and the fraction organic carbon (f_{oc}) in the soil and aquifer.

The metals modeling methodology in EPACMTP incorporates two options to specify the K_d for a given metal. Adsorption isotherms for metals with nonlinear sorption behavior are computed using EPA's geochemical speciation model, MINTEQA2 (Allison et al., 1991); and the isotherms for metals which cannot be accurately modeled with MINTEQA2 are specified as pH dependent empirical relationships (Loux et al., 1990). The two approaches for calculating the K_d values are described briefly below; more detailed information can be found in U.S. EPA (1996c and 1997a).

In the first approach, the purpose of using the MINTEQA2 model is to capture the variation in K_d due to variability in geochemical conditions in the soil and changing dissolved metal concentrations. The four geochemical parameters on which adsorption is assumed to primarily depend are: groundwater pH, concentration of hydrous ferric oxide adsorption sites, concentration of dissolved and particulate natural organic matter, and concentration of leachate organic acids. For the MINTEQA2 modeling, the natural variability of these parameters is divided into three ranges: low, medium, and high. Then, each parameter was assigned three possible values, which correspond approximately to the midpoint of each range. For each metal with nonlinear adsorption, the MINTEQA2 model was then run over a range of total metal concentrations to produce an isotherm for each combination of the three possible values for the four geochemical parameters. For each metal, the 162 isotherms produced in this way were then written to a data file that must accompany the input file when conducting EPACMTP modeling. EPACMTP then selects the appropriate isotherm based on the input values specified for the four geochemical parameters.

To perform geochemical modeling with MINTEQA2, one must know the adsorption reactions describing the interaction of the metal with the adsorbing surface. For several metals of concern, primarily those that behave as anions in aqueous solution, these reactions are not reliably known. Because the MINTEQA2 model could not be used due to this lack of data, a second approach was developed that uses empirical linear relationships to describe the adsorption distribution coefficient as a function of pH. The pH-dependent isotherms were determined from statistical analysis of laboratory measurements of soil and aquifer materials and corresponding groundwater and leachate samples (Loux et al., 1990). These isotherms are included in the EPACMTP code, and the appropriate K_d value is calculated based on the input value specified for groundwater pH in the unsaturated and saturated zones.

Deterministic Modeling For The Chlorinated Aliphatics Listing Determination

The risk analysis for the chlorinated aliphatics listing determination consists of three phases of modeling for the landfill and land treatment unit scenarios: a deterministic sensitivity analysis, a deterministic 2-parameter high end analysis, and a probabilistic analysis. The first two phases will be described in this section.

The sensitivity analysis is used to identify and rank the most influential variables in the analysis. For the chlorinated aliphatics listing determination, the sensitivity analysis was conducted in deterministic mode; that is, each input is set to a constant value, one model realization is performed, and the model outputs one receptor well concentration. Additionally, this sensitivity analysis separately evaluated the influence of each of a number of input parameters. The first step of the sensitivity analysis was to run EPACMTP with all input parameters set to their respective central tendency (median) values. Then, one at a time, each input to be examined in the sensitivity analysis was set to its high end (usually the 10th or the 90th percentile) value and the variation in the receptor well concentration from the central tendency case is noted. The inputs having the greatest impact on the receptor well concentration are identified as the most sensitive parameters. Note that the highest 9 or 30-year average receptor well concentration is used for carcinogenic constituents and the highest 9-year average receptor well concentration is used for non-carcinogenic constituents.

The two most sensitive parameters identified in the sensitivity analysis are then set to their respective high end values in the high end analysis, while the remaining parameters are set to their median values. The resulting receptor well concentration is defined as the high end concentration.

Deterministic Sensitivity Analysis

The purpose of the groundwater pathway sensitivity analysis is to identify the most sensitive parameters in the exposure and risk calculations, and their corresponding high end and central tendency values for the subsequent deterministic analysis. The sensitivity of individual parameters is defined as the difference, or ratio, in predicted health risk when the parameter is set to its high end value, compared to the risk corresponding to the central tendency value of that parameter. The high end value of a parameter corresponds to its 90th percentile value or its 10th percentile value, depending on whether a high or a low value of that parameter results in a higher predicted risk. If there is limited data to define the probability distribution of a parameter, the high end may be set to either the maximum or minimum measured value. The central tendency value corresponds to the 50th percentile (median) value of the parameter.

Identification and Description of Important Parameters

The various parameters can be grouped into constituent-related parameters, waste- and WMU-related parameters, pathway-related parameters, and intake-related parameters. This discussion does not include all parameters in the groundwater model or in the exposure and risk equations, but is restricted to those that are expected to be among the most sensitive parameters.

Constituent-related Parameters. The most important parameters in this group are:

- Concentration of constituent in the waste
- Concentration of constituent in the leachate
- Organic carbon partition coefficient (for organics), or the solid-liquid partition coefficient (for metals and inorganics)
- Transformation (hydrolysis) half-life

For the landfill scenario, the constituent-specific leachate concentration was included in the sensitivity analysis and was based on industry-specific sampling data. For dioxins, the Toxicity Characteristic Leaching Procedure (TCLP) concentration for sample OG-04 was used as the central tendency value, and the TCLP concentration for sample GL-01 was used as the high end value for leachate concentration. For all other constituents, the central tendency value for leachate concentration was calculated as the average TCLP concentration and the high end value was defined as the maximum TCLP concentration.

However, the constituent-specific waste concentration was not included in the sensitivity analysis for landfills because the TCLP data did not necessarily correspond to the mean and max waste concentration. Note that waste concentration data have been compiled based on dry weights and wet weights; the wet weight concentrations are lower than the dry weight concentrations. The effect of varying waste concentration is similar to that of waste volume (which was included in the sensitivity analysis); increasing either of these parameters will increase the leaching duration, and drive the exposure concentration at the receptor well toward a steady state value. For the dioxins, the dry weight waste concentration for sample OG-04 was used as the central tendency value, and the dry weight waste concentration for sample GL-01 was used as the high end value for waste concentration. For bis(2-chloroethyl)ether, 2-(2-chloroethoxy)ethanol, 1,4-dioxane, and arsenic the average wet weight values from industry-specific sampling data were used for waste concentration. For all other constituents, the constituent-specific value for waste concentration was calculated as the average dry weight waste concentration. Since the dry weight concentrations are higher than the wet weight concentrations, and since no constituents for which the analysis was performed based on dry weight concentrations showed excessive risk, these analyses were not repeated using wet weight concentrations.

For the land treatment unit scenario, leachate concentration is an input for the groundwater model, but waste concentration is not. The groundwater model uses the conservative assumption that during operation of the LTU, the source is periodically replenished through additional waste applications, so that no significant depletion of the source occurs. In other words, the leachate concentration emanating from the LTU remains constant. The magnitude of the leachate concentration in this scenario is controlled by the waste concentration, as determined by the source partitioning model. The effect of waste concentration was, therefore, included in the modeling analysis, but this parameter was not used as a separate model input parameter. Central tendency and high end leachate concentration values were modeled by varying the waste concentration in the partitioning model from its central tendency value to its high end value, respectively.

The last two constituent-specific parameters, partition coefficient (k_d) or organic carbon partition coefficient (k_{oc}), and the hydrolysis half-life, are considered to be properties of the constituents which do not generally vary. Thus, these parameters were not considered in the sensitivity analysis.

Waste and Waste Management Unit-Related Parameters. Landfills and land treatment units are the two types of waste management units (WMUs) that were evaluated in this risk assessment. The significant parameters in this category include:

- WMU surface area
- Infiltration rate through the WMU
- WMU operating life
- Annual waste amount

The product of WMU area and infiltration rate equals the annual volumetric leachate flux through the WMU. The product of leachate flux times leachate concentration equals the annual mass of constituent that is released into the subsurface. For a given WMU area and leachate concentration, a higher infiltration rate means a higher loading of contaminant into the soil and groundwater, but, for the landfill scenario, also a more rapid depletion of the constituent. Assuming a uniform WMU design (earthen cover, no liner), the infiltration rate is controlled by climatic factors, i.e., it will vary depending on the geographic location of the waste management unit.

The landfill operating life and the annual quantity of waste disposed determine the total amount of waste that accumulates in the landfill. Landfill operating life was not varied in the sensitivity analysis because 30 years has been defined as the average operating life for municipal landfills (U.S. EPA, 1997b).

For the land treatment unit scenario, the constituent is assumed to leach into the subsurface at a constant rate and at a constant concentration during the active life of the unit. After the unit no longer accepts sludge for land application, it is assumed that the amount of leachate generated will quickly diminish. Thus, it was conservatively assumed that after cessation of sludge application, the generation of leachate would continue for no more than 40 years. Adding these 40 years of leaching after unit closure to the assumed 40 years of active use of the land application unit produces the leaching duration of 80 years for this waste disposal scenario. Thus, land application unit active life and leaching duration were not varied in the sensitivity analysis.

The annual waste quantity is characterized by considerable uncertainty and variation; therefore, this parameter was examined in the sensitivity analysis.

Groundwater Pathway Related Parameters. The most important parameters affecting dilution and attenuation in the soil and groundwater include:

- Soil type and soil characteristics (including saturated conductivity and water content)
- Depth to groundwater
- Saturated zone thickness
- Aquifer hydraulic conductivity
- Hydraulic gradient
- Distance to nearest receptor well
- Depth of well intake point
- Position of well relative to plume centerline

In support of the 1995 HWIR proposal, a methodology and database were developed to relate a number of the most important soil and groundwater parameters to waste unit location (U.S. EPA 1997a and 1997b). These location-dependent parameters are: (1) depth to groundwater, (2) saturated zone thickness, (3) aquifer hydraulic conductivity, and (4) hydraulic gradient. These data were used for this modeling analysis to determine the value of each of these parameters at each facility location modeled.

Whereas distance to nearest receptor well and position of the well relative to plume centerline were examined in the sensitivity analysis, depth of well intake point was not included. There can be significant differences in groundwater concentration at different depths below the water table. However, the depth at which the maximum concentration occurs varies according to well location and the hydrogeologic setting being modeled. Therefore, for the sensitivity analysis, the well was placed at the vertical mid-point of the aquifer.

It is important to note that the dilution and attenuation of waste constituents during transport in the groundwater pathway depends strongly on the pathway-related parameters identified above and on the constituent-specific sorption (k_d or k_{oc}) parameters and hydrolysis transformation rate. The effect of sorption (high k_{oc} or k_d) is to retard the movement of constituents relative to the rate of groundwater movement, thereby increasing the travel time through both the unsaturated zone (from the base of the landfill to the water table) and the saturated zone to the receptor well.

For constituents that do not hydrolyze, the primary effect of this retardation is to delay the time of maximum exposure. For relatively large waste volumes (in which contaminant transport approaches steady state conditions), the magnitude of the exposure at the receptor well is less affected. For smaller waste volumes, the magnitude of the exposure at the receptor well may be significantly affected by retardation. For constituents that do hydrolyze, an increased travel time means that a greater proportion of the constituent mass will have transformed before it reaches the receptor well, which may result in lower exposure and risk (although the risk associated with toxic transformation daughter products may be increased). Thus, the relative sensitivity of "depth to groundwater" and "distance to receptor well" may be markedly different for different constituents.

Intake Related Parameters. Parameters in this category include:

- Exposure duration (for carcinogens only)
- Exposure frequency
- Groundwater intake (ingestion) rate
- Body weight

The sensitivity analysis includes evaluation of both modeling parameters and intake-related parameters. Since the risk equation is linear, these intake parameters can be evaluated directly, without the use of groundwater modeling. For instance, if all other factors remain constant, a doubling of the ingestion rate doubles the risk. Moreover, the parameters in this group generally act independently of any of the other parameters discussed before (all of which affect the exposure concentration), and are generally independent of the constituent being analyzed.

Exposure duration, applicable for carcinogens only, is the exception to these generalizations. Exposure duration is the most sensitive of the intake-related parameters; its central tendency value is 9 years, and its high end value is 30 years for adult residents (U.S. EPA, 1997c). In order to maintain consistency between the modeled groundwater transport scenario and the risk analysis scenario, exposure duration was examined in the sensitivity analysis for carcinogenic constituents. Given a constant receptor well concentration, increasing the exposure duration (from 9 years to 30 years) for carcinogens increases risk by slightly more than a factor of 3 (the ratio of 30 to 9).

Since the ratio of high end receptor well concentration to central tendency well concentration for the first most sensitive parameter is greater than 3, the ratio for the second most sensitive parameter was calculated and compared to that of exposure duration. If the ratio for the second most sensitive parameter is greater than three, then it was chosen as the second parameter for the high end analysis and the central tendency value of 9 years was used for exposure duration. Conversely, if the ratio for the second most sensitive parameter is less than 3, then exposure duration (30 years) was chosen as the second parameter for the high end analysis. For non-carcinogens, the peak receptor well concentration was always used.

Summary of Simulation Procedure

The sensitivity of individual parameters is defined as the difference, or ratio, in predicted health risk when the parameter is set to its high end value, compared to the risk corresponding to the central tendency value of that parameter. The high end value of a parameter corresponds to its 90th percentile value or its 10th percentile value, depending on whether a high or a low value of that parameter results in a more conservative (higher) predicted risk. If there is limited data to define the probability distribution of a parameter, the high end may be set to either the maximum or minimum measured value. The central tendency value corresponds to the 50th percentile (median) value of the parameter.

The sensitivity analysis was conducted by performing a number of modeling runs for each constituent. First, all parameters were set to their central tendency values. Then one at a time, each parameter was set to its high end value while all the other parameters remained at their central tendency values. These values and the data sources for the landfill scenario and the land treatment unit scenario are presented in Appendix K. The list of parameters examined in the sensitivity analysis for landfills and land treatment units are presented in Tables D.4-1 and D.4-2. The modeling results were then tabulated, and the parameters, including intake parameters, were ranked in order of sensitivity for each group of constituents. Finally, the two most sensitive parameters were identified for use in the subsequent deterministic analysis. The complete groundwater modeling results for the sensitivity analysis are presented in Appendix H. These results are summarized here in Tables D.4-3 and D.4-4. Note that cis-1,3-dichloropropene and dioxins did not reach the receptor well. The neutral hydrolysis rate constant and K_{oc} used to model cis-1,3-dichloropropene were 40 yr^{-1} and 63.1 cm^3/g, respectively (Kollig 1993). Data for dioxins are presented in Appendix C.

Table D.4-1. Parameters Examined in the Sensitivity Analysis for the Landfill Scenario

Landfill Parameters
X-well
Y-well
Area
Site Location
Leachate Concentration
Waste Volume
Exposure Duration (carcinogens only)

Table D.4-2. Parameters Examined in the Sensitivity Analysis for the Land Treatment Unit Scenario

Land Treatment Unit Parameters
Leachate Concentration
X-well
Y-well
Exposure Duration (carcinogens only)

Table D.4-3. Results of Sensitivity Analysis for Landfill Scenario

Constituent of Concern	Two Most Sensitive Parameters
1,2-Dichloroethane	X-well and Area
Chloroform	X-well and Area
Methylene chloride	X-well and Exposure Duration
cis-1,3-Dichloropropene	Not determined [a]
OCDD	Not determined [a]
OCDF	Not determined [a]
1,2,3,4,7,8,9-HpCDF	Not determined [a]
1,2,3,4,6,7,8-HpCDF	Not determined [a]
Bis(2-chloroethyl)ether	Site Location and X-well
2-(2-chloroethoxy)ethanol	Site Location and X-well
1,4-Dioxane	X-well and Area
Arsenic	X-well and Exposure Duration
Manganese	X-well and Area
Molybdenum	X-well and Waste Volume
Nickel	Site Location and X-well

[a] The relative sensitivity of the parameters could not be determined because the plume did not reach the receptor well for the central tendency scenario or any of the high end scenarios.

Table D.4-4. Results of Sensitivity Analysis for Land Treatment Unit Scenario

Constituent of Concern	Two Most Sensitive Parameters
Arsenic	Leachate Concentration and Exposure Duration
Bis(2-chloroethyl)ether	X-well and Exposure Duration
2-(2-chloroethoxy)ethanol	X-well and Exposure Duration
1,4-Dioxane	X-well and Exposure Duration

Deterministic Analysis

The purpose of the groundwater pathway deterministic analysis for the chlorinated aliphatics waste streams is to predict the potential chemical-specific high end and central tendency risks for the landfill and land treatment unit scenarios. The RME scenario is defined by setting the two most sensitive parameters to their respective high end values and setting all other parameters to their central tendency values. In addition, a deterministic central tendency analysis, in which all parameters are set to their central tendency values, was performed.

Linkage of Partitioning Model and EPACMTP

The source model developed by RTI was used to simulate the major fate and transport processes, such as leaching, hydrolysis, and volatilization, that occur within the waste management unit. The partitioning model and the EPACMTP model can be run sequentially, as long as all parameters that are common to both models, e.g. landfill area and infiltration rate, are set to the same values in both models. If this is not done, then conservation of contaminant mass is not maintained.

For the landfill scenario, the partitioning model was used to predict the reduction in constituent amount due to volatilization during the active life of the unit. The waste concentration used for the groundwater pathway modeling for the landfill scenario was adjusted to account for these volatilization losses. The TCLP concentration was used as the initial leaching concentration for the landfill scenario.

For the land treatment unit scenario, the partitioning model was used to generate a leachate profile for each constituent to be modeled; that is, a history of the annual average leachate concentrations. To be conservative, the maximum 9-year average leachate concentration during the 80 years after the opening of the unit was used as the leachate concentration for the land treatment unit scenario.

Results of the Deterministic Analysis

Some constituents did not reach the receptor well within the 10,000 year modeling period for any of the high end scenarios; thus, for these constituents, a two-parameter high end analysis was not conducted. These constituents are cis-1,3-Dichloropropene, OCDD, OCDF, 1,2,3,4,7,8,9-HpCDF, and 1,2,3,4,6,7,8-HpCDF and are generally characterized by very high K_{OC} values. The EPACMTP model would predict that they are only very slowly mobile in the subsurface. The results of the deterministic central tendency and high end analysis for the landfill and land treatment unit scenarios for the remaining constituents are presented below in Tables D.4-5 and D.4-6.

Table D.4-5. Results of the Deterministic Analysis for the Landfill Scenario

Constituent of Concern	Scenario	Receptor Well Concentration (mg/L)
1,2-Dichloroethane	Central Tendency	8.85E-05
	High end X-well and Area	1.26E-03
Chloroform	Central Tendency	1.16E-04
	High end X-well and Area	1.03E-03
Methylene chloride	Central Tendency	1.43E-04
	High end X-well and Exposure Duration	8.98E-04
Bis(2-chloroethyl)ether	Central Tendency	1.19E-07
	High end Site Location and X-well	1.30E-04
2-(2-chloroethoxy)ethanol	Central Tendency	2.82E-07
	High end Site Location and X-well	7.29E-04
1,4-Dioxane	Central Tendency	1.12E-04
	High end X-well and Area	1.46E-03
Arsenic	Central Tendency	2.10E-04
	High end X-well and Exposure Duration	1.42E-03
Manganese	Central Tendency	1.18E-01
	High end X-well and Area	1.55E+00
Molybdenum	Central Tendency	2.48E-04
	High end X-well and Waste Volume	4.75E-03
Nickel	Central Tendency	1.62E-06
	High end Site Location and X-well	3.08E-01

Table D.4-6. Results of the Deterministic Analysis for the Land Treatment Unit Scenario

Constituent of Concern	Scenario	Receptor Well Concentration (mg/L)
Arsenic	Central Tendency	1.88E-04
	High end Leachate Concentration and Exposure Duration	5.00E-04
Bis(2-chloroethyl)ether	Central Tendency	4.45E-06
	High end X-well and Exposure Duration	1.16E-05
2-(2-chloroethoxy)ethanol	Central Tendency	1.08E-05
	High end X-well and Exposure Duration	2.39E-05
1,4-Dioxane	Central Tendency	2.84E-05
	High end X-well and Exposure Duration	4.73E-05

Probabilistic Modeling For The Chlorinated Aliphatics Listing Determination

The purpose of the groundwater pathway Monte Carlo analysis is to provide a probabilistic estimate of risk given the uncertainty and variability in groundwater pathway parameters. The Monte Carlo analysis also provides an estimate of where in the distribution of risk the results of the deterministic analysis fall.

For this analysis, the output of the groundwater fate and transport model is a probability distribution of receptor well concentrations. The Monte Carlo analysis was only conducted for constituents which showed significant (for example, greater than $1x10^{-6}$) risk in the high end deterministic analysis. For the landfill scenario, these constituents were bis(2-chloroethyl)ether, 2-(2-chloroethoxy)ethanol, 1,4-dioxane, and arsenic. For the land treatment unit, arsenic was the only constituent for which the Monte Carlo modeling was performed.

The resulting groundwater concentrations for the Monte Carlo analysis are presented in Appendix H.

Monte Carlo Modeling Methodology

As in the deterministic analysis, each constituent was modeled individually. The landfill partitioning model was used to adjust the waste concentration to account for volatilization losses which occur prior to installation of the landfill cap. The land treatment unit partitioning model was used to conservatively estimate the constituent concentration in the leachate which infiltrates into the subsurface. The output of the partitioning models, the landfill waste concentration and the land treatment unit leachate concentration, in turn, were provided as input to the EPACMTP subsurface fate and transport model, which then calculated the corresponding average exposure concentrations at a specified groundwater receptor well (U.S. EPA, 1997a and 1997b).

In the deterministic analysis, the creation of model input files and assignment of parameter values was done manually. In a Monte Carlo analysis, which involves 2,000 model simulations (realizations), parameter values were drawn randomly from appropriate probability distributions; a process which is fully automated in both the source partitioning model and in EPACMTP. The models must be synchronized to the extent that the same values for common parameters are used in each individual Monte Carlo realization. The values for the common modeling parameters were saved for each Monte Carlo realization of the partitioning models along with the calculated output concentrations. These values were then used as input for the subsequent Monte Carlo groundwater pathway modeling using EPACMTP. The above procedure was implemented to maintain conservation of mass in a Monte Carlo analysis.

The Monte Carlo methodology is summarized here for the landfill and land treatment unit scenarios. A detailed discussion of the site-based methodology and data sources for the probability distributions of the input parameters and a detailed discussion of how the partitioning models and EPACMTP were linked in the Monte Carlo analysis are presented in Appendix F.

For the landfill scenario, the partitioning model was used to predict the reduction in constituent amount due to volatilization during the active life of the unit. The waste concentration used for the groundwater pathway modeling for the landfill scenario was adjusted to account for these volatilization losses. Note that the TCLP concentration was used as the initial leaching concentration in the groundwater modeling for the landfill scenario.

For a given constituent, the landfill partitioning model was used to adjust the waste concentration to account for pre-emplacement volatilization losses. The partitioning model was run for 1,000 realizations, and after each realization, the inputs and the resulting output waste concentration were saved to an ASCII data file. This data file was then used as input to the EPACMTP groundwater fate and transport model. For each realization of the subsequent groundwater pathway Monte Carlo analysis, EPACMTP picked a random record from the file generated by the source partitioning model; the model then read in the values of the common input parameters in that record. The hydrogeologic region and climate region indices were then employed to choose random values for other saturated and unsaturated zone parameters appropriate to the landfill location associated with the chosen record. For each of the 2,000 EPACMTP Monte Carlo realizations, the receptor well concentration of interest, e.g., either the peak concentration or the maximum 9-year average concentration, was then calculated and saved to an output file. At the conclusion of the modeling, a probability distribution function for the receptor well concentrations was constructed. This distribution of concentrations was then used as one of the inputs in the Monte Carlo analysis of risk.

For the land treatment unit scenario, the partitioning model was used to generate a leachate history for arsenic (the only constituent to be modeled); that is, a history of the annual average leachate concentrations. To be conservative, the maximum 9-year average leachate concentration during the 80 years after the opening of the unit was used as the leachate concentration in the groundwater modeling for the land treatment unit scenario. Note that waste concentration is not a model input for the land treatment unit.

For arsenic, the land treatment unit partitioning model was used to generate the leachate concentration infiltrating to the subsurface. The partitioning model was run for 1,000 realizations, and after each realization, the inputs and the resulting output leachate concentration were saved to an ASCII data file. This data file was then used as input to the EPACMTP groundwater fate and transport model. For each realization of the subsequent groundwater pathway Monte Carlo analysis, EPACMTP picked a random record from the file generated by the source partitioning model; the model then read in the values of the common input parameters in that record. Since there is only one land treatment unit location, the hydrogeologic region and climate region indices were set to constant values. Random numbers generated by the model were employed to choose random values for saturated and unsaturated zone parameters from the distributions appropriate to this location. For each of the 2,000 EPACMTP Monte Carlo realizations, the maximum 9-year average receptor well concentration was then calculated and saved to an output file. At the conclusion of the modeling, a probability distribution function for the receptor well concentrations was constructed. This distribution of concentrations was then used as one of the inputs in the Monte Carlo analysis of risk.

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Appendix D.5

Surface Water Model

Appendix D.5

Surface Water Model

Introduction

The framework for estimating surface water impacts from the management of chlorinated aliphatics wastes is based on the methodology presented in *Addendum to Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions* (U.S. EPA, 1993), henceforth referred to as the Addendum. The model estimates water column and bed sediment concentrations. Fish tissue concentrations are estimated from water column or sediment concentrations using bioconcentration factors (BCFs), bioaccumulation factors (BAFs), or biota-sediment accumulation factors (BSAFs).

Water column concentrations include dissolved, sorbed to suspended sediments, and total concentration (sorbed plus dissolved). The model accounts for six routes of contaminant entry into the waterbody: (1) contaminant sorbed to eroding soils, (2) contaminant dissolved in runoff, (3) particle-bound contaminant deposition, (4) wet deposition of vapor phase contaminant, (5) direct diffusion of vapor phase contaminants, and (6) discharge of contaminated groundwater. The model also accounts for processes that remove contaminants. These include: volatilization of dissolved phase contaminants from the water column and contaminant removal via burial. The impact to the waterbody is assumed to be uniform, which is more realistic for smaller waterbodies than for larger ones. Key assumptions in the model include the following:

- Soil concentrations within the depositional area are uniform

- Concentrations within the surface soils, sediments, suspended solids, and water can be described by partition coefficients

- At equilibrium, gaseous diffusion into the water equals volatilization from the water

- Equilibrium is maintained between contaminants within the water column and contaminants in sediment (this is established when the dissolved phase concentration within the bed sediments is equal to the dissolved phase concentration in the water column)

- Rate of contaminant burial in bed sediments is estimated as a function of the sediment deposition rate.

Waterbody/Watershed Characterization

The parameters contained in this section characterize the surface waterbody (a stream) simulated by the model. The waterbody characterization parameters are another example of a set of parameters that are interdependent; therefore, they are set and varied as a group.

Van der Leeden et al. (1990) ranked over 2 million streams located throughout the United States according to their stream order. A first-order stream has no tributary channels; a second-order stream forms when two first-order streams converge, and so on through stream order 10. Each successive stream order is characterized by a larger flow volume. For each stream order, van der Leeden presented typical values for flow, waterbody area, watershed area, depth, and various other parameters. The central tendency and high-end waterbody were characterized by selecting a central tendency and high-end stream order and using van der Leeden's typical values for the chosen stream order. A stream smaller than the central tendency stream was desired for high end, since a smaller stream will dilute contaminants discharged into it less than a larger stream. Van der Leeden's data are reproduced in Table D.5-1.

Stream orders 1 and 2 are typically too small to sustain an appreciable amount of aquatic life for fishing and were therefore eliminated from consideration. Of the stream orders sufficiently large to support aquatic life for fishing (stream orders 3 through 10), stream order 5 was selected as representative of central tendency stream characteristics, based on the number of streams in the United States that have streams of each stream order. There was a significant drop in the number of streams between stream orders 5 and 6. It appeared that the number of streams in the United States that could be classified as stream order 6 or above was too small to be used to represent a national average or central tendency. However, a significant number of streams fell into stream order classification 5. Because a smaller stream was needed for high end, stream order 3, the smallest that would support significant aquatic life, was selected to characterize a high-end stream.

Table D.5-2 summarizes the stream data used to characterize the central tendency and high-end waterbodies. These values have been converted to metric units, as needed by the model. Watershed area (called drainage area by van der Leeden), flow, depth, and velocity were taken directly from van der Leeden. Waterbody area was calculated from average length and width. Flow-independent mixing volume was calculated from average length, width, and depth, as suggested in the Addendum.

The surface water model requires three different depth measurements as inputs: depth of the water column, depth of bed sediment, and total waterbody depth (which is the sum of the water column and sediment depths). The depth from van der Leeden was for total waterbody depth. The Addendum suggests a typical bed sediment depth of 0.03 m; this was used, and the water column depth calculated as the difference between the total waterbody depth from van der Leeden and the bed sediment depth of 0.03 m.

Table D.5-1. Summary of U.S. Stream Data

Stream order	Number of streams	Total length (mi)	Average length (mi)	Drainage area (mi^2)	Surface area (mi^2)	Mean flow (ft^3/s)	Mean width (ft)	Mean depth (ft)	Mean velocity (ft/s)
1	1,570,000	1,570,000	1.0	1.0	1,200	0.65	4	0.15	1.0
2	350,000	810,000	2.1	4.7	1,500	3.1	10	0.29	1.3
3	80,000	420,000	5.3	23	1,400	15	18	0.58	1.5
4	18,000	220,000	12	109	1,500	71	37	1.1	1.8
5	4,200	116,000	28	518	1,600	340	75	2.2	2.3
6	950	61,000	64	2,500	1,800	1,600	160	4.1	2.7
7	200	30,000	147	12,000	1,800	7,600	320	8.0	3.3
8	41	14,000	338	56,000	1,700	36,000	650	15	3.9
9	8	6,200	777	260,000	1,500	171,000	1,300	29	5.6
10	1	1,800	1,800	1,250,000	1,000	810,000	2,800	55	5.9

Source: Van der Leeden et al. (1990).

Table D.5-2. Characterization of Central Tendency and High-End Waterbodies

Parameter	Central tendency	High-end
Stream order	5	3
Watershed area	1.3e+9 m^2	6e+7 m^2
Flow	3e+8 m^3/yr (3e+11 L/yr)	1.3e+7 m^3/yr (1.3e+10 L/yr)
Velocity	0.7 m/s	0.5 m/s
Depth (waterbody)	0.67 m	0.18 m
Width	23 m	5.5 m
Length	45,000 m	8,500 m
Waterbody area (length × width)	1e+6 m^2	4.6e+4 m^2
Flow-independent mixing volume (length × width × depth)	6.7e+5 m^3 (6.7e+8 L)	8.3e+3 m^3 (8.3e+6 L)
Depth (bed sediment)	0.03 m	0.03 m
Depth (water column)	0.64 m	0.15 m

Other Surface Water Parameters

Total Suspended Solids

The Addendum suggests that total suspended solids (TSS) can range from 1 to 100 mg/L and suggests a typical value of 10 mg/L for streams and rivers. This value is used as the central tendency value. A higher value was needed for high end. No data on frequency of values in actual streams were available to estimate a 90th percentile value. The Addendum suggests that 80 mg/L is a cutoff value for protection of aquatic life; this is also toward the high end of the range suggested. Therefore, 80 mg/L is used as a high-end value.

Bed Sediment Concentration

The bed sediment concentration term is analogous to the bulk density for soil in that it describes the concentration of solids in terms of a mass per unit volume. The Addendum notes that bed sediment concentration should range from 0.5 to 1.5 kg/L and that a reasonable value for most applications is 1 kg/L. The range suggested was sufficiently narrow; thus, no advantage would be gained by setting a high-end value for this parameter; therefore the value suggested of 1 kg/L (1e+6 mg/L) is used.

Bed Sediment Porosity

The bed sediment porosity describes the volume of water per volume of benthic space. Bed sediment porosity is calculated from bed sediment concentration and sediment density as follows (Addendum):

$$\theta_{bs} = 1 - \frac{BS}{\rho_s} \qquad \text{(D.5-1)}$$

where

θ_{bs} = bed sediment porosity (L/L)
BS = bed sediment concentration = 1 kg/L = 1,000,000 mg/L
ρ_s = sediment density = 2.65 kg/L (a standard value for mineral materials).

This results in a value of 0.6. As with bed sediment concentration, this value is used for both the central tendency and high-end.

Gas-Phase Transfer Coefficient

The gas-phase transfer coefficient is used to estimate volatile losses from the waterbody. Volatile losses are calculated using a two-layer resistance model that incorporates a gas-phase transfer coefficient and a liquid-phase transfer coefficient. Both transfer coefficients are controlled by flow-induced turbulence in flowing systems. The liquid-phase transfer coefficient is calculated based on chemical-specific properties as specified in the Addendum. The

Addendum gives a single value for the gas-phase transfer coefficient for flowing systems of 36,500 m/yr. This value is used and is not varied.

There is some uncertainty around setting this parameter to a single value that is not chemical specific. It is reasonable to assume that chemical properties affecting volatility would have some effect on this value, although it is not known how large such an effect would be. The Addendum does give an equation (using chemical-specific properties) for calculating this parameter for stagnant systems, such as lakes or ponds. However, the transfer coefficients for stagnant systems are dominated by wind-induced turbulence rather than flow-induced turbulence; therefore, this equation is not applicable to flowing systems such as are modeled here and is not used.

Fraction Organic Carbon in Bottom Sediment

The fraction organic carbon in bottom sediment is derived from the fraction organic carbon in watershed soils. This value is site-specific and the same value is used for the waterbody as is used for the nonwaterbody soils.

Waterbody Temperature

An average surface waterbody temperature of 298 K (25°C) was considered a "common assumption for water temperature" in the Addendum. Although this value is somewhat high, the results are insensitive to this parameter, and reasonable lower values should have no effect on the results; therefore, this parameter is not varied. This temperature value was used to estimate gaseous diffusion loads into the surface waterbody.

Fish Concentrations

Fish were assumed to be exposed to chlorinated aliphatic waste constituents through water column and bed sediment in the waterbodies. The contaminants in the water column consist of dissolved constituents and constituents associated with suspended solids. For metals, the dissolved fraction is more significant and is the most bioavailable form. The equations used to estimate surface water concentrations are presented in Appendix E of this document. The results of these equations are used to estimate the concentration of contaminants in fish; the concentrations in fish tissue are estimated using compound-specific BCFs, BAFs, or BSAFs.

Bioconcentration is defined as the net uptake of a chemical from an organism’s surrounding medium through direct contact (e.g., uptake by a fish through the gills) but excluding ingestion of a chemical in food. Bioaccumulation is defined as the net uptake of a chemical from the environment from all pathways (including direct contact and ingestion of contaminated food). It is important to recognize that the distinction between BCF and BAF has both practical and technical implications. The route of exposure assumed for BCFs is direct contact, and BCF values are typically generated from controlled laboratory studies where fish are exposed to the chemical only through water. For organic chemicals with log K_{ow} values below ~4.0, the BCF provides a reasonable estimate of the concentration expected to be found in fish under field conditions. However, for more hydrophobic organic chemicals (log K_{ow} >> 4.0), uptake via the food chain will be an increasingly important source of exposure and using a BCF will tend to underestimate the concentration in fish tissue. Therefore, for hydrophobic organic chemicals, and other chemicals shown to bioaccumulate (e.g., mercury), a BAF is the preferred factor to use for estimating fish tissue concentrations. BAFs are typically generated from field studies or estimated from models.

In addition to the distinction between BCFs and BAFs, it is important to recognize the difference between dissolved water concentrations versus total water concentrations. For organic chemicals with log K_{ow} below 4.0, chemical concentrations in water are typically regarded as freely dissolved, although some small fraction will be adsorbed to suspended particles. In contrast, for metals and hydrophobic organic chemicals having low solubility, water concentrations are generally regarded as total water concentrations (i.e., freely dissolved and particle-bound). Because the freely dissolved fraction is considered to be the bioavailable fraction, it is important to distinguish between freely dissolved and total water concentrations when estimating BCFs and BAFs as well as when conducting fate and transport modeling. Dissolved water concentrations were used for most of the organic chemicals and mercury. Total water concentrations were used for pentachlorophenol, bis(2-ethylhexyl)phthalate, and di-n-octyl phthalate.

The following equations are used to estimate fish tissue concentrations of metals and organics (except dioxins) in freshwater:

$$C_{fish} = C_w \ x \ BAF \qquad \text{(D.5-2)}$$

or

$$C_{fish} = C_w \ x \ BCF \qquad \text{(D.5-3)}$$

where

C_{fish} = fish concentration (mg/kg)
C_w = water concentration (mg/L)
BAF = bioaccumulation factor (L/kg)
BCF = bioconcentration factor (L/kg).

BSAFs were used to characterize the accumulation of dioxins into fish tissue. A BSAF is a similar measure of uptake to BCFs or BAFs, but it is calculated based on concentrations of the constituent in sediment rather than the water column. A BSAF assumes equilibrium between sediment, pore water, and the water column. When partitioning of constituents between sediments, particles, pore water, and surface water are accounted for, good correlation between BSAFs and surface-water-derived BAFs is noted.

In the freshwater ecosystem, 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) can bioaccumulate in fish even though concentrations of TCDD in the water column are below detection. Hence, calculating BAFs based on surface water concentrations introduces greater uncertainty. Given these limitations (the accuracy of TCDD measurement and BAF estimation), use of surface water concentrations may misrepresent actual bioaccumulation. However, extremely hydrophobic constituents, such as dioxin congeners, can be measured more easily in sediments and aquatic life because these dioxin and furan congeners tend to partition into organic carbon in the sediment and into fish lipids once taken into the organism. For these reasons, biological uptake factors that reflect the relationship between sediment concentrations and organism concentrations, such as BSAF, may be more appropriate to characterize food chain transfer of these constituents. Consequently, the BSAF is the preferred metric for estimating accumulation for dioxin congeners. The following equation was used to estimate dioxin concentrations in fish tissue:

$$C_{fish} = \frac{C_{sed} \, x \, BSAF \, x \, f_{lipid}}{f_{oc}} \tag{D.5-4}$$

where

C_{fish} = fish concentration (mg/kg)
C_{sed} = sediment concentration (mg/kg)
BSAF = biota-sediment bioaccumulation (kg/kg)
f_{lipid} = lipid content of fish (unitless)
f_{oc} = fraction organic carbon in bottom sediment (unitless).

References

U.S. EPA (Environmental Protection Agency). 1993. *Addendum to Methodology for Assessing Health Risks Associated with Indirect Exposure to Comubstor Emissions*. EPA/600/AP-93003. Office of Health and Environmental Assessment, Washington, DC.

Van der Leeden, F., F.L. Troise, and D.K. Todd. 1990. *The Water Encyclopedia*. 2nd ed. Chelsea, MI: Lewis Publishers.

Appendix E

Indirect and Direct Exposure Equations

Appendix E

Indirect and Direct Exposure Equations

Table E-1.1. Constituent Concentration in Residential Plot Due to Erosion

Adult Resident Exposure Scenario

$$C_R = \frac{SL_{0,F}\ x\ C_0\ x\ ER}{ks_R\ x\ M_R} + \frac{SL_{B,F}\ x\ C_{B/Surr}\ x\ ER}{M_R\ x\ ks_R} + \frac{Ds_{(1)R}}{ks_R}$$

Parameter	Definition	Central Tendency	High End
C_R	Constituent concentation at residential plot (mg/kg)		
$SL_{0,F}$	Soil load delivered to off-site location for material originating in source area (kg/yr)	Calculated (see Table E-1.2.)	
$SL_{B,F}$	Soil load delivered to off-site location for material originating in buffer area (kg/yr)	Calculated (see Table E-1.7.)	
$C_{B/Surr}$	Constituent concentration in buffer and surrounding areas (mg/kg)	Calculated (see Table E-1.11.)	
$Ds_{(1),R}$	Deposition term for the residential plot (mg/kg-yr)	Calculated (see Table E-1.24.)	
C_0	Source contaminant concentration (mg/kg)	Chemical-specific	
ks_R	Constituent loss constant from the residential plot (1/yr)	Calculated (see Table E-1.25.)	
M_R	Mass of soil in mixing depth of residential plot (kg)	Calculated (see Table E-1.32.)	
ER	Constituent enrichment ratio (unitless)	Organics = 3 Metals = 1	

Description

This equation is used to calculate the mass of constituent deposited onto a residential plot as a result of erosion from the source.

Table E-1.2. Soil Load Delivered to Off-Site Location for Material Originating from Source Area

All Exposure Scenarios

$$SL_{0,F} = X_{e,S} \times A_S \times (1 - SD_{SB}) \times SF_{0,F}$$

Parameter	Definition	Central Tendency	High End
$SL_{0,F}$	Soil load delivered to off-site location for material originating from source area (kg/yr)		
$X_{e,S}$	Unit soil loss from source (kg/m^2-yr)	Calculated (see Table E-1.3.)	
A_S	Area of source (m^2)	Source-specific	
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)	Calculated (see Table E-1.4.)	
$SF_{0,F}$	Scaling factor	Calculated (see Table E-1.6.)	

Description

This equation is used to calculate the load of eroded soil, originating from the source, and is deposited onto the off-site location of interest.

Table E-1.3. Universal Soil Loss Equation (USLE) for the Source Area

All Exposure Scenarios

$$X_{e,S} = R_S \ x \ K_S \ x \ LS_S \ x \ C_S \ x \ P_S \ x \ \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,S}$	Unit soil loss from the source (kg/m^2-yr)		
R_S	USLE rainfall (or erosivity) factor (1/yr)	Site Specific	
K_S	USLE erodibility factor (ton/acre)	Site Specific	
LS_S	USLE length-slope factor (unitless)	Site Specific	
C_S	USLE cover management factor (unitless)	Site Specific	
P_S	USLE supporting practice factor (unitless)	Site Specific	
907.18	Conversion factor (kg/ton)		
4047	Conversion factor (m^2/acre)		

Description

This equation calculates the soil loss rate from the source using the Universal Soil Loss Equation; the result is used in the soil erosion load equation.

Table E-1.4. Sediment Delivery Ratio

All Exposure Scenarios

$$SD_{SB} = a \; x \; (A_S + A_{B/Surr} + A_F)^{-b}$$

Parameter	Definition	Central Tendency	High End
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)		
a	Empirical intercept coefficient	Depends on subbasin area; see table below	
A_S	Area of source (m^2)	Waste management scenario specific	
$A_{B/Surr}$	Area of buffer and surrounding areas (m^2)	Calculated (see Table E-1.5.)	
A_F	Area of off-site location of interest (m^2)	Ag. field = 2,000,000 Residential plot or home garden = 5,100	
b	Empirical slope coefficient	0.125	

Description

This equation calculates the sediment delivery ratio for the sub-basin; the result is used in the soil erosion load equation.

Values for Empirical Intercept Coefficient, a

Sub-basin (A_s+$A_{B/Surr}$+A_F)	"a" coefficient (unitless)
≤ 0.1	2.1
1	1.9
10	1.4
100	1.2
1,000	0.6
1 sq. mile = 2.59×10^6 m^2	

Table E-1.5. Buffer and Surrounding Areas

All Exposure Scenarios

$$A_{B/Surr} = d_b \; x \; \sqrt{A_F} \quad if \quad A_F > A_S$$

$$A_{B/Surr} = (\sqrt{A_F} + d_b) \; x \; \sqrt{A_S} - \sqrt{A_F} \;\; if \;\; A_S \geq A_F \;\; but \;\; \sqrt{A_S} < d_b + \sqrt{A_F}$$

$$A_{B/Surr} = A_S - A_F \;\; if \;\; A_S > A_F \;\; and \;\; \sqrt{A_S} \geq d_b + \sqrt{A_F}$$

Parameter	Definition	Central Tendency	High End
$A_{B/Surr}$	Area of buffer and surrounding areas (m^2)		
d_b	Distance between source and field (side length of buffer area) (m)	Scenario Specific	
A_F	Area of off-site location of interest (m^2)	Ag field = 2,000,000 Residential plot or home garden = 5,100	
A_S	Area of source (m^2)	Waste management of scenario-specific	

Description

This equation calculates the area of the buffer and surrounding areas for each of the different exposure scenarios.

Table E-1.6. Scaling Factor

All Exposure Scenarios

$$SF_{0,F} = \frac{A_F}{A_S + A_{B/Surr} + A_F}$$

Parameter	Definition	Central Tendency	High End
$SF_{0,F}$	Scaling factor		
A_F	Area of off-site location of interest (m^2)	Ag. field = 2,000,000 Residential or home garden = 5,100	
$A_{B/Surr}$	Area of buffer and surrounding area (m^2)	Calculated (see Table E-1.5.)	
A_S	Area of source (m^2)	Waste management scenario-specific	

Description

This term is used to determine what portion of the total amount of eroded source material available for deposition within the sub-basin will be deposited onto the off-site location of interest.

Table E-1.7. Soil Load Delivered to Off-Site Location for Material Originating from Buffer Area

All Exposure Scenarios

$$SL_{B,F} = X_{e,B} \; x \; A_B \; x \; (1 - SD_{SB}) \; x \; SF_{B,F}$$

Parameter	Definition	Central Tendency	High End
$SL_{B,F}$	Soil load delivered to off-site location for material originating from buffer area (kg/yr)		
$X_{e,B}$	Unit soil loss from buffer area (kg/m^2-yr)	Calculated (see Table E-1.8.)	
A_B	Area of buffer (m^2)	Calculated (see Table E-1.9.)	
SD_{SB}	Sediment delivery ratio for sub basin (unitless)	Calculated (see Table E-1.4.)	
$SF_{B,F}$	Scaling factor	Calculated (see Table E-1.10.)	

Description

This equation is used to calculate the load of eroded soil originating from the buffer area and is deposited onto the off-site location of interest.

Table E-1.8. Universal Soil Loss Equation (USLE) for Buffer Area

All Exposure Scenarios

$$X_{e,B} = R_B \ x \ K_B \ x \ LS_B \ x \ C_B \ x \ P_B \ x \ \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,B}$	Unit soil loss for buffer area (kg/m^2 -yr)		
R_B	USLE rainfall factor (1/yr)	Site Specific	
K_B	USLE erodibility factor (ton/acre)	Site Specific	
LS_B	USLE length-slope factor (unitless)	Site Specific	
C_B	USLE cover factor (unitless)	Site Specific	
P_B	USLE erosion control practice factor (unitless)	Site Specific	
907.18	Units conversion factor (kg/ton)		
4047	Units conversion factor (m^2/acre)		

Description

This equation is used to calculate the soil loss rate from the buffer area using the Universal Soil Loss Equation; the result is used in the soil erosion load equation.

Table E-1.9. Buffer Area

All Exposure Scenarios

$$A_B = d_b \, x \, \sqrt{A_F} \quad if \quad A_F > A_S$$

$$A_B = d_b \, x \, \sqrt{A_S} \quad if \quad A_S \geq A_F$$

Parameter	Definition	Central Tendency	High End
A_B	Area of buffer (m^2)		
d_b	Distance between source and field (side-length of buffer area) (m)	Scenario Specific	
A_F	Area of off-site location of interest (m^2)	Ag. Field = 2,000,000 Residential plot or home garden = 5,100	
A_S	Area of source (m^2)	Waste management scenario-specific	

Description

This equation calculates the area of the buffer.

Table E-1.10. Scaling Factor

All Exposure Scenarios

$$SF_{B,F} = \frac{A_F}{A_{B/Surr} + A_F}$$

Parameter	Definition	Central Tendency	High End
$SF_{B,F}$	Scaling factor		
A_F	Area of off-site location (m^2)	Ag. field = 2,000,000 Residential plot or home garden = 5,100	
$A_{B/Surr}$	Area of buffer and surrounding area (m^2)	Calculated (see Table E-1.5.)	

Description

This term is used to determine what portion of the total amount of eroded buffer material, available for deposition within the sub-basin, will be deposited onto the off-site location of interest.

Table E-1.11. Constituent Concentration in Buffer and Surrounding Areas Due to Erosion

All Exposure Scenarios

$$C_{B/Surr} = \frac{SL_{0,B/Surr}\ x\ C_0\ x\ ER}{ks_{B/Surr}\ x\ M_{B/Surr}} + \frac{Ds_{(1),B/Surr}}{ks_{B/Surr}}$$

Parameter	Definition	Central Tendency	High End
$C_{B/Surr}$	Constituent concentration in the buffer and surrounding area (mg/kg)		
$SL_{0,B/Surr}$	Soil load delivered to buffer and surrounding area (kg/yr)	Calculated (see Table E-1.12.)	
C_0	Source constituent concentration (mg/kg)	Chemical-specific	
$ks_{B/Surr}$	Constituent loss constant for buffer and surrounding area (1/yr)	Calculated (see Table E-1.15.)	
$M_{B/Surr}$	Mass of soil in mixing depth of buffer area (kg)	Calculated (see Table E-1.23.)	
$Ds_{(1), B/Surr}$	Deposition term for off-site field (mg/kg-yr)	Calculated (see Table E-1.14.)	
ER	Constituent enrichment ratio (unitless)	Organics = 3 Metals = 1	

Description

This equation is used to calculate the constituent concentration in the buffer and surrounding areas as a result of erosion from the source.

Table E-1.12. Soil Load Delivered to Buffer and Surrounding Area for Material Originating from Source

All Exposure Scenarios

$$SL_{0,B/Surr} = X_{e,S} \ x \ A_S \ x \ (1 - SD_{SB}) \ x \ SF_{0,B/Surr}$$

Parameter	Definition	Central Tendency	High End
$SL_{0,B/Surr}$	Soil load delivered to buffer and surrounding area (kg/yr)		
$X_{e,S}$	Unit soil loss from source (kg/m^2-yr)	Calculated (see Table E-1.3.)	
A_S	Area of source (m^2)	Source-specific	
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)	Calculated (see Table E-1.4.)	
$SF_{0,B/Surr}$	Scaling factor	Calculated (see Table E-1.13.)	

Description

This equation is used to calculate the load of eroded soil originating from the source and is deposited onto the buffer and surrounding areas.

Table E-1.13. Scaling Factor

All Exposure Scenarios

$$SF_{0,B/Surr} = \frac{A_{B/Surr}}{A_S + A_{B/Surr} + A_F}$$

Parameter	**Definition**	**Central Tendency**	**High End**
$SF_{0,B/Surr}$	Scaling factor		
A_F	Area of off-site location (m^2)	Ag. field = 2,000,000 Residential plot or home garden = 5,100	
$A_{B/Surr}$	Area of buffer and surrounding area (m^2)	Calculated (see Table E-1.5.)	
A_S	Area of source (m^2)	Waste management scenario-specific	

Description

This term is used to determine what portion of the total amount of eroded source material, available for deposition within the sub-basin, will be deposited onto the buffer and surrounding areas.

Table E-1.14. Deposition Rate Factor to Buffer and Surrounding Areas

All Exposure Scenarios

$$Ds_{(1),B/Surr} = \frac{100 \, x \, Q}{Z_{B/Surr} \, x \, BD} \, x \, [F_v \, (0.31536 \, x \, Vdv_F \, x \, Cyv_F + Dywv_F) + (Dydp_F + Dywp_F) \, x \, (1 - F_v)]$$

Parameter	Definition	Input Value
$Ds_{(1),B/Surr}$	Deposition term for buffer and surrounding areas (mg/kg-yr)	
100	Units conversion factor ([mg-m^2]/[kg-cm^2])	
Q	Source emissions (g/sec)	Waste mgt. scenario-specific
$Z_{B/Surr}$	Soil mixing depth of buffer and surrounding areas - untilled (cm)	2.5
BD	Soil bulk density (g/cm^3)	Site Specific
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific (U.S. EPA 1993)
0.31536	Units conversion factor (m-g-s/cm-µg-yr)	
Vdv_F	Dry deposition velocity for field (cm/s)	0.2
Cyv_F	Normalized vapor phase air concentration for field (µg-s/g-m^3)	Modeled ISC3
$Dywv_F$	Normalized yearly wet deposition from vapor phase for field (s/m^2-yr)	Modeled ISC3
$Dydp_F$	Normalized yearly dry deposition from particle phase for field (s/m^2-yr)	Modeled ISC3
$Dywp_F$	Normalized yearly wet deposition from particle phase for field (s/m^2-yr)	Modeled ISC3

Description

This equation calculates average air deposition occurring over the exposure duration as a result of wet and dry deposition of particles onto soil, deposition of wet vapors onto soil, and diffusion of dry vapors into soil. Contaminants are assumed to be incorporated only to a finite depth (the mixing depth, Z). The air deposition rates (per unit area) for the buffer and surrounding areas are assumed to be the same as the air deposition rates (per unit area) to the field.

Table E-1.15. Constituent Loss Constant

All Exposure Scenarios

$$ks_{B/Surr} = ksl_{B/Surr} + kse_{B/Surr} + ksr_{B/Surr} + ksg_{B/surr} + ksv_{B/Surr}$$

Parameter	Definition	Central Tendency	High End
$ks_{B/Surr}$	Constituent loss constant due to all processes for the buffer and surrounding areas (1/yr)		
$ksl_{B/Surr}$	Constituent loss constant due to leaching (1/yr)	Calculated (see Table E-1.16.)	
$kse_{B/Surr}$	Constituent loss constant due to soil erosion (1/yr)	Calculated (see Table E-1.19.)	
$ksr_{B/Surr}$	Constituent loss constant due to surface runoff (1/yr)	Calculated (see Table E-1.21.)	
$ksg_{B/Surr}$	Constituent loss constant due to degradation (1/yr)	Chemical Specific	
$ksv_{B/Surr}$	Constituent loss constant due to volatilization (1/yr)	Calculated (see Table E-1.22.)	

Description

This equation calculates the constitutent loss constant, which accounts for the loss of constituent from soil by multiple mechanisms.

Table E-1.16. Constituent Loss Constant Due to Leaching

All Exposure Scenarios

$$ksl_{B/Surr} = \frac{P + I - R - E_v}{\theta \; x \; Z_{B/Surr} \; x \; [1.0 + (BD \; x \; Kd_s / \theta)]}$$

Parameter	Definition	Central Tendency	High End
$ksl_{B/Surr}$	Constituent loss constant for buffer and surrounding area due to leaching (1/yr)		
P	Average annual precipitation (cm/yr)	Site Specific	
I	Average annual irrigation (cm/yr)	0	
R	Average annual runoff (cm/yr)	Site Specific	
E_v	Average annual evapotranspiration (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
$Z_{B/Surr}$	Soil depth of buffer and surrounding area from which leaching removal occurs - untilled (cm)	2.5	
BD	Soil bulk density (g/cm^3)	Site Specific	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	

Description

This equation calculates the constituent loss constant due to leaching from soil.

Table E-1.17. Soil Volumetric Water Content

All Exposure Scenarios

$$\theta = \theta_s \left[\frac{q}{K_s} \right]^{\left(\frac{1}{2b+3} \right)}$$

Parameter	Definition	Central Tendency	High End
θ	Soil volumetric water content (mL/cm^3)		
θ_s	Soil saturated volumetric water content (mL/cm^3)	Site Specific	
q	Average annual recharge rate (cm/yr)	Calculated (see Table E-1.18.)	
K_s	Saturated hydraulic conductivity (cm/yr)	Site Specific	
b	Soil-specific exponent representing water retention (unitless)	Site Specific	

Description

This equation calculates the volumetric water content of the soil

Table E-1.18. Average Annual Recharge

All Exposure Scenarios

$$q = P + I - E_v - R$$

Parameter	Definition	Central Tendency	High End
q	Average annual recharge rate (cm/yr)		
P	Average annual precipitation (cm/yr)	Site Specific	
I	Average annual irrigation (cm/yr)	0	
E_v	Average annual evapotranspiration (cm/yr)	Site Specific	
R	Average annual runoff (cm/yr)	Site Specific	

Description

This equation calculates the average annual groundwater recharge rate.

Table E-1.19. Constituent Loss Constant Due to Erosion

All Exposure Scenarios

$$kse_{B/Surr} = \frac{0.1 \ x \ ER \ x \ X_{e,B/Surr} x \ [SD_{SB} + (1 - SD_{SB})(\frac{A_F}{A_{B/Surr} + A_F})]}{BD \ x \ Z_{B/Surr}} \ x \ \left(\frac{Kd_s \ x \ BD}{\theta + (Kd_s \ x \ BD)} \right)$$

Parameter	Definition	Central Tendency	High End
$kse_{B/Surr}$	Constituent loss constant for buffer and surrounding area due to soil erosion (1/yr)	Calculated	
$X_{e,B/Surr}$	Unit soil loss for buffer and surrounding area (kg/m^2-yr)	Calculated (see Table E-1.20.)	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
$Z_{B/Surr}$	Soil mixing depth for buffer and surrounding area - untilled (cm)	2.5	
BD	Soil bulk density (g/cm^3)	Site Specific	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
SD_{SB}	Sediment delivery ratio for the sub-basin (unitless)	Calculated (see Table E-1.4).	
ER	Constituent enrichment ratio (unitless)	Organics = 3 Metals - 1	
A_F	Area of off-site location (m^2)	Ag. Field = 2,000,000 Residential plot or home garden = 5,100	
$A_{B/Surr}$	Area of buffer and surrounding areas (m^2)	Calculated (See Table E-1.5.)	

Description

This equation is used to calculate the constituent loss constant from the buffer and surrounding area due to erosion

Table E-1.20. Universal Soil Loss Equation (USLE) for Buffer and Surrounding Areas

All Exposure Scenarios

$$X_{e,B/Surr} = R_{B/Surr} \times K_{B/Surr} \times LS_{B/Surr} \times C_{B/Surr} \times P_{B/Surr} \times \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,B/Surr}$	Unit soil loss for buffer and surrounding area (kg/m^2 -yr)		
$R_{B/Surr}$	USLE rainfall factor (1/yr)	Site Specific	
$K_{B/Surr}$	USLE erodibility factor (ton/acre)	Site Specific	
$LS_{B/Surr}$	USLE length-slope factor (unitless)	Site Specific	
$C_{B/Surr}$	USLE cover factor (unitless)	Site Specific	
$P_{B/Surr}$	USLE erosion control practice factor (unitless)	Site Specific	
907.18	Units conversion factor (kg/ton)		
4047	Units conversion factor (m^2/acre)		

Description

This equation is used to calculate the soil loss rate from the buffer and surrounding area using the Universal Soil Loss Equation; the result is used in the soil erosion load equation.

Table E-1.21. Constituent Loss Constant Due to Runoff

All Exposure Scenarios

$$ksr_{B/Surr} = \frac{R}{\theta \times Z_{B/Surr}} \times \left(\frac{1}{1 + (Kd_s \times BD/\theta)} \right)$$

Parameter	Definition	Central Tendency	High End
$ksr_{B/Surr}$	Constituent loss constant for buffer and surrounding area due to runoff (1/yr)		
R	Average annual runoff (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.))	
$Z_{B/Surr}$	Soil mixing depth of buffer and surrounding area - untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific (see Table 3-4)	
BD	Soil bulk density (g/cm^3)	Site Specific	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-1.22. Constituent Loss Constant Due to Volatilization

All Exposure Scenarios

$$ksv_{B/Surr} = \left[\frac{3.1536x10^{7}\,x\,H}{Z_{B/Surr}\,x\,Kd_{s}\,x\,R\,x\,T\,x\,BD}\right] x \left[0.482\,x\,u^{0.78}\,x\left(\frac{\mu_{a}}{\rho_{a}\,x\,D_{a}}\right)^{-0.67} x\left(\sqrt{\frac{4\,x\,A_{B/Surr}}{\pi}}\right)^{-0.11}\right]$$

Parameter	Definition	Central Tendency	High End
$ksv_{B/Surr}$	Constituent loss constant for buffer and surrounding area due to volatilization (1/yr)		
$3.1536x10^{7}$	Conversion constant (s/yr)		
H	Henry's law constant (atm-m^3/mol)	Chemical-specific	
$Z_{B/Surr}$	Soil mixing depth of buffer and surrounding area - untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
R	Universal gas constant (atm-m^3/mol-K)	$8.205x10^{-5}$	
T	Ambient air temperature (K)	Site Specific	
BD	Soil bulk density (g/cm^3)	Site Specific	
u	Average annual windspeed (m/s)	Site Specific	
μ_a	Viscosity of air (g/cm-s)	$1.81x10^{-4}$	
ρ_a	Density of air (g/cm^3)	$1.2x10^{-3}$	
D_a	Diffusivity of constituent in air (cm^2/s)	Chemical-specific	
$A_{B/Surr}$	Area of buffer and surrounding areas (m^2)	Calculated (see Table E-1.5.)	

Description

This equation calculates the constituent loss constant due to volatilization from soil.

Source: IEM.

Table E-1.23. Mass of Soil in Mixing Depth of Buffer and Surrounding Areas

All Exposure Scenarios

$$M_{B/Surr} = Z_{B/Surr} \; x \; A_{B/Surr} \; x \; BD \, x \; 10$$

Parameter	Definition	Central Tendency	High End
$M_{B/Surr}$	Mass of soil in mixing depth of buffer and surrounding area (kg)		
$Z_{B/Surr}$	Soil mixing depth for buffer and surrounding area - untilled (cm)	2.5	
$A_{B/Surr}$	Area of buffer and surrounding areas (m^2)	Calculated (see Table E-1.5.)	
BD	Soil bulk density (g/cm^3)	Site Specific	
10	Units conversion factor		

Description

This equation is used to calculate the total mass of soil in the buffer and surrounding areas that will be mixed with the mass of eroded material.

Table E-1.24. Deposition Rate Factor to Residential Plot from Source

Adult Resident Exposure Scenario

$$Ds_{(1),R} = \frac{100 \, x \, Q}{Z_R \, x \, BD} \, x \, [\cong (0.31536 \, x \, Vdv_F \, x \, Cyv_F + Dywv_F) + (Dydp_F + Dywp_F) \, x \, (1 - F_v)]$$

Parameter	Definition	Input Value
$Ds_{(1),R}$	Deposition term for residental plot - Adult Resident (mg/kg-yr)	
100	Units conversion factor ([mg-m^2]/[kg-cm^2])	
Q	Source emissions (g/s)	Waste mgt. scenario-specific
Z_R	Soil mixing depth of residential plot - untilled (cm)	2.5
BD	Soil bulk density (g/cm^3)	Site Specific
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific
0.31536	Units conversion factor (m-g-s/cm-µg-yr)	
Vdv_F	Dry deposition velocity for field (cm/s)	0.2
Cyv_F	Normalized vapor phase air concentration for field (µg-s/g-m^3)	Modeled ISC3
$Dywv_F$	Normalized yearly wet deposition from vapor phase for field (s/m^2-yr)	Modeled ISC3
$Dydp_F$	Normalized yearly dry deposition from particle phase for field (s/m^2-yr)	Modeled ISC3
$Dywp_F$	Normalized yearly wet deposition from particle phase for field (s/m^2-yr)	Modeled ISC3

Description

This equation calculates average air deposition occurring over the exposure duration as a result of wet and dry deposition of particles onto soil, deposition of wet vapors onto soil, and diffusion of dry vapors into soil. Contaminants are assumed to be incorporated only to a finite depth (the mixing depth, Z).

Table E-1.25. Constituent Loss Constant

Adult Resident Exposure Scenario

$$ks_R = ksl_R + kse_R + ksr_R + ksg_R + ksv_R$$

Parameter	Definition	Central Tendency	High End
ks_R	Constituent loss constant due to all processes from resident plot - Adult Resident (1/yr)		
ksl_R	Constituent loss constant due to leaching (1/yr)	Calculated (see Table E-1.26.)	
kse_R	Constituent loss constant due to soil erosion (1/yr)	Calculated (see Table E-1.27.)	
ksr_R	Constituent loss constant due to surface runoff (1/yr)	Calculated (see Table E-1.30.)	
ksg_R	Constituent loss constant due to degradation (1/yr)	Chemical Specific	
ksv_R	Constituent loss constant due to volatilization (1/yr)	Calculated (see Table E-.31..)	

Description

This equation calculates the constituent loss constant, which accounts for the loss of constituent from soil by multiple mechanisms.

Table E-1.26. Constituent Loss Constant Due to Leaching

Adult Resident Exposure Scenario

$$ksl_R = \frac{P + I - R - E_v}{\theta \ x \ Z_R \ x \ [1.0 + (BD \ x \ Kd_s/\theta)]}$$

Parameter	Definition	Central Tendency	High End
ksl_R	Constituent loss constant from residential plot due to leaching - Adult Resident (1/yr)		
P	Average annual precipitation (cm/yr)	Site Specific	
I	Average annual irrigation (cm/yr)	0	
R	Average annual runoff (cm/yr)	Site Specific	
E_v	Average annual evapotranspiration (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_R	Soil depth for residential plot which leaching removal occurs - untilled (cm)	2.5	
BD	Soil bulk density (g/cm^3)	Site Specific	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	

Description

This equation calculates the constituent loss constant due to leaching from soil.

Table E-1.27. Constituent Loss Constant Due to Erosion

Adult Resident Exposure Scenario

$$kse_R = \frac{0.1 \ x \ ER \ x \ X_{e,R} \ x \ [SD_{SB} + (1 - SD_{SB})(\frac{A_{BF}}{A_F \ + \ A_{BF}})]}{BD \ x \ Z_R} \ x \ \left(\frac{Kd_s \ x \ BD}{\theta + (Kd_s \ x \ BD)} \right)$$

Parameter	Definition	Central Tendency	High End
kse_R	Constituent loss constant due to erosion for residential plot - Adult Resident (1/yr)		
$X_{e,R}$	Unit soil loss from the residential plot (kg/m^2-yr)	Calculated (see Table E-1.28.)	
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)	Calculated (see Table E-1.4.)	
ER	Contaminant enrichment ratio (unitless)	Organics = 3 Metals = 1	
BD	Soil bulk density (g/cm^3)	Site Specific	
Z_R	Soil mixing depth of residential plot - untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
A_F	Area of residential plot (m^2)	Residential plot = 5,100	
A_{BF}	Buffer area between residential plot and waterbody (m^2)	Calculated (see Table E-1.29..)	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-1.28. Universal Soil Loss Equation (USLE) for Residential Plot

Adult Resident Exposure Scenario

$$X_{e,R} = R_R \ x \ K_R \ x \ LS_R \ x \ C_R \ x \ P_R \ x \ \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,R}$	Unit soil loss from the residential plot (kg/m^2 -yr)		
R_R	USLE rainfall factor (1/yr)	Site Specific	
K_R	USLE erodibility factor (ton/acre)	Site Specific	
LS_R	USLE length-slope factor (unitless)	Site Specific	
C_R	USLE cover factor (unitless)	Site Specific	
P_R	USLE erosion control practice factor (unitless)	Site Specific	
907.18	Units conversion factor (kg/ton)		
4047	Units conversion factor (m^2/acre)		

Description

This equation is used to calculate the soil loss rate from the residential plot using the Universal Soil Loss Equation.

Table E-1.29. Area of Buffer Between Field and Waterbody

All Exposure Scenarios

$$A_{BF} = 0 \qquad if \quad \sqrt{A_S} \le d_b + \sqrt{A_F}$$

$$A_{BF} = \sqrt{A_F}\ x\ (\sqrt{A_S} - d_b - \sqrt{A_F}) \qquad if\ \sqrt{A_S} > d_b + \sqrt{A_F}$$

Parameter	Definition	Central Tendency	High End
A_{BF}	Area of buffer between field and waterbody (m^2)		
A_F	Area of field (m^2)	Ag. Field = 2,000,000 Residential plot or home garden = 5,100	
A_S	Area of source (m^2)	Waste management scenario-specific	
d_b	Distance between source and field (side-length of buffer area) (m)	Scenario Specific	

Description

This equation calculates the area of the buffer between the field and the waterbody.

Table E-1.30. Constituent Loss Constant Due to Runoff

Adult Resident Exposure Scenario

$$ksr_R = \frac{R}{\theta x Z_R} x \left(\frac{1}{1 + (Kd_s x BD/\theta)} \right)$$

Parameter	Definition	Central Tendency	High End
ksr_R	Constituent loss constant due to runoff for residential plot - Adult Resident (1/yr)		
R	Average annual runoff (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_R	Soil mixing depth of residential plot - untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
BD	Soil bulk density (g/cm^3)	Site Specific	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-1.31. Constituent Loss Constant Due to Volatilization

Adult Resident Exposure Scenario

$$ksv_R = \left[\frac{3.1536x10^7 \, x \, H}{Z_R \, x \, Kd_s \, x \, R \, x \, T \, x \, BD}\right] x \left[0.482 \, x \, u^{0.78} \, x \left(\frac{\mu_a}{\rho_a \, x \, D_a}\right)^{-0.67} x \left(\sqrt{\frac{4 \, x \, A_R}{\pi}}\right)^{-0.11}\right]$$

Parameter	Definition	Central Tendency	High End
ksv_R	Constituent loss constant due to volatilization from residential plot - Adult Resident (1/yr)		
$3.1536x10^7$	Conversion constant (s/yr)		
H	Henry's law constant (atm-m^3/mol)	Chemical-specific	
Z_R	Soil mixing depth of residential plot - untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
R	Universal gas constant (atm-m^3/mol-K)	$8.205x10^{-5}$	
T	Ambient air temperature (K)	Site Specific	
BD	Soil bulk density (g/cm^3)	Site Specific	
u	Average annual windspeed (m/s)	Site Specific	
μ_a	Viscosity of air (g/cm-s)	$1.81x10^{-4}$	
ρ_a	Density of air (g/cm^3)	$1.2x10^{-3}$	
D_a	Diffusivity of constituent in air (cm^2/s)	Chemical-specific	
A_R	Area of residential plot (m^2)	5,100	

Description

This equation calculates the constituent loss constant due to volatilization from soil.

Table E-1.32. Mass of Soil in Mixing Depth of Residential Plot

Adult Resident Exposure Scenario

$$M_R = Z_R \ x \ A_R \ x \ BD \ x \ 10$$

Parameter	Definition	Central Tendency	High End
M_R	Mass of soil in mixing depth of residential plot - Adult Resident (kg)		
Z_R	Soil mixing depth for residential plot - untilled (cm)	2.5	
A_R	Area of residential plot (m^2)	5,100	
BD	Soil bulk density (g/cm^3)	Site Specific	
10	Units conversion factor		

Description

This equation is used to calculate the total mass of soil in the residential plot that will be mixed with the mass of eroded material.

Table E-2.1. Concentration in Home Garden Due to Erosion

Home Gardener Exposure Scenario

$$C_{HG} = \frac{SL_{0,F} \ x \ C_0 \ x \ ER}{ks_{HG} \ x \ M_{HG}} + \frac{SL_{B,F} \ x \ C_{B/Surr} \ x \ ER}{ks_{HG} \ x \ M_{HG}} + \frac{Ds_{(1),HG}}{ks_{HG}}$$

Parameter	Definition	Central Tendency	High End
C_{HG}	Constituent concentration in home garden (mg/kg)		
$SL_{0,F}$	Soil load delivered to off-site location for material originating in source area (kg/yr)	Calculated (see Table E-1.2.)	
$SL_{B,F}$	Soil load delivered to off-site location for material originating in buffer area (kg/yr)	Calculated (see Table E-1.7.)	
$C_{B/Surr}$	Constituent concentration in buffer and surrounding areas (mg/kg)	Calculated (see Table E-1.11)	
$Ds_{(1),HG}$	Deposition term for the home garden (mg/kg-yr)	Calculated (see Table E-2.9.)	
C_0	Source constituent concentration (mg/kg)	Chemical-specific	
ks_{HG}	Constituent loss constant from the home garden (1/yr)	Calculated (see Table E-2.2.)	
ER	Constituent enrichment ratio (unitless)	organics = 3 metals = 1	
M_{HG}	Mass of soil in mixing depth of home garden (kg)	Calculated (see Table E-2.8.)	

Description

This equation is used to calculate the mass of constituent deposited onto the home garden as a result of erosion from the source.

Table E-2.2. Constituent Loss Constant

Home Gardener Exposure Scenario

$$ks_{HG} = ksl_{HG} + kse_{HG} + ksr_{HG} + ksg_{HG} + ksv_{HG}$$

Parameter	Definition	Central Tendency	High End
ks_{HG}	Constituent soil loss constant due to all processes from home garden (1/yr)		
ksl_{HG}	Constituent loss constant due to leaching (1/yr)	Calculated (see Table E-2.3.)	
kse_{HG}	Constituent loss constant due to soil erosion (1/yr)	Calculated (see Table E-2.4)	
ksr_{HG}	Constituent loss constant due to surface runoff (1/yr)	Calculated (see Table E-2.6.)	
ksg_{HG}	Constituent loss constant due to degradation (1/yr)	Chemical Specific	
ksv_{HG}	Constituent loss constant due to volatilization (1/yr)	Calculated (see Table E-2.7.)	

Description

This equation calculates the constituent loss constant, which accounts for the loss of constituent from soil by multiple mechanisms.

Table E-2.3. Constituent Loss Constant Due to Leaching

Home Gardener Exposure Scenario

$$ksl_{HG} = \frac{P + I - R - E_v}{\theta \; x \; Z_{HG} \; x \; [1.0 + (BD \; x \; Kd_s/\theta)]}$$

Parameter	Definition	Central Tendency	High End
ksl_{HG}	Constituent loss constant due to leaching for home gardener (1/yr)		
P	Average annual precipitation (cm/yr)	Site Specific	
I	Average annual irrigation (cm/yr)	0	
R	Average annual runoff (cm/yr)	Site Specific	
E_v	Average annual evapotranspiration (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_{HG}	Soil depth of home garden from which leaching removal occurs – tilled (cm)	20	
BD	Soil bulk density (g/cm^3)	Site Specific	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	

Description

This equation calculates the constituent loss constant due to leaching from soil.

Table E-2.4. Constituent Loss Constant Due to Erosion

Home Gardener Exposure Scenario

$$kse_{HG} = \frac{0.1 \ x \ ER \ x \ X_{e,HG} \, x \, [SD_{SB} + (1 - SD_{SB})(\frac{A_{BF}}{A_F \, + \, A_{BF}})]}{BD \ x \ Z_{HG}} \ x \ \left(\frac{Kd_s \ x \ BD}{\theta + (Kd_s \ x \ BD)} \right)$$

Parameter	Definition	Central Tendency	High End
kse_{HG}	Constituent loss constant due to erosion for home gardener (1/yr)		
$X_{e,HG}$	Unit soil loss from the home garden (kg/m^2-yr)	Calculated (see Table E-2.5.)	
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)	Calculated (see Table E-1.4.)	
ER	Constituent enrichment ratio (unitless)	Organics = 3 Metals = 1	
BD	Soil bulk density (g/cm^3)	Site Specific	
Z_{HG}	Soil mixing depth of home garden – tilled (cm)	20	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
A_{HG}	Area of home garden (m^2)	5,100	
A_{BF}	Buffer area between home garden and waterbody (m^2)	Calculated (see Table E-1.29.)	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-2.5. Universal Soil Loss Equation (USLE) for Home Garden

Home Gardener Exposure Scenario

$$X_{e,HG} = RF_{HG} \times K_{HG} \times LS_{HG} \times C_{HG} \times P_{HG} \times \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,HG}$	Unit soil loss from home garden (kg/m^2-yr)		
RF_{HG}	USLE rainfall factor (1/yr)	Site Specific	
K_{HG}	USLE erodibility factor (ton/acre)	Site Specific	
LS_{HG}	USLE length-slope factor (unitless)	Site Specific	
C_{HG}	USLE cover management factor (unitless)	Site Specific	
P_{HG}	USLE erosion control practice factor (unitless)	Site Specific	
907.18	Conversion factor (kg/ton)		
4047	Conversion factor (m^2/acre)		

Description

This equation is used to calculate the soil loss rate from the home garden using the Universal Soil Loss Equation.

Table E-2.6. Constituent Loss Constant Due to Runoff

Home Gardener Exposure Scenario

$$ksr_{HG} = \frac{R}{\theta\, x\, Z_{HG}}\, x \left(\frac{1}{1 + (Kd_s\, x\, BD/\theta)} \right)$$

Parameter	Definition	Central Tendency	High End
ksr_{HG}	Constituent loss constant due to runoff for home gardener (1/yr)		
R	Average annual runoff (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_{HG}	Soil mixing depth of home garden – tilled (cm)	20	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
BD	Soil bulk density (g/cm^3)	Site Specific	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-2.7. Constituent Loss Constant Due to Volatilization

Home Gardener Exposure Scenario

$$ksv_{HG} = \left[\frac{3.1536 x 10^{7}\, x\, H}{Z_{HG}\, x\, Kd_{s}\, x\, R\, x\, T\, x\, BD}\right] x \left[0.482\, x\, u^{0.78}\, x \left(\frac{\mu_{a}}{\rho_{a}\, x\, D_{a}}\right)^{-0.67} x \left(\sqrt{\frac{4\, x\, A_{HG}}{\pi}}\right)^{-0.11}\right]$$

Parameter	Definition	Central Tendency	High End
ksv_{HG}	Constituent loss constant due to volatilization for home gardener (1/yr)		
$3.1536x10^{7}$	Conversion constant (s/yr)		
H	Henry's law constant (atm-m^{3}/mol)	Chemical-specific	
Z_{HG}	Soil mixing depth of home garden – tilled (cm)	20	
Kd_{s}	Soil-water partition coefficient (cm^{3}/g)	Chemical-specific	
R	Universal gas constant (atm-m^{3}/mol-K)	$8.205x10^{-5}$	
T	Ambient air temperature (K)	Site Specific	
BD	Soil bulk density (g/cm^{3})	Site Specific	
u	Average annual windspeed (m/s)	Site Specific	
μ_{a}	Viscosity of air (g/cm-s)	$1.81x10^{-4}$	
ρ_{a}	Density of air (g/cm^{3})	$1.2x10^{-3}$	
D_{a}	Diffusivity of constituent in air (cm^{2}/s)	Chemical-specific	
A_{HG}	Area of home garden (m^{2})	5,100	

Description

This equation calculates the constituent loss constant due to volatilization from soil.

Table E-2.8. Mass of Soil in Mixing Depth of Home Garden

Home Gardener Exposure Scenario

$$M_{HG} = Z_{HG} \; x \; A_{HG} \; x \; BD \; x \; 10$$

Parameter	Definition	Central Tendency	High End
M_{HG}	Mass of soil in mixing depth of home garden (kg)		
Z_{HG}	Soil mixing depth for home garden – tilled (cm)	20	
A_{HG}	Area of home garden (m^2)	5,100	
BD	Soil bulk density (g/cm^3)	Site Specific	
10	Units conversion factor		

Description

This equation is used to calculate the total mass of soil in the home garden that will be mixed with the mass of eroded material.

Table E-2.9. Deposition Rate Factor to Home Garden from Source

Home Gardener Exposure Scenario

$$Ds_{(1),HG} = \frac{100 \, x \, Q}{Z_{HG} \, x \, BD} \, x \, [F_v \, (0.31536 \, x \, Vdv_{HG} \, x \, Cyv_{HG} + Dywv_{HG}) + (Dydp_{HG} + Dywp_{HG}) \, x \, (1 - F_v)]$$

Parameter	Definition	Input Value
$Ds_{(1),HG}$	Deposition term for home garden (mg/kg-yr)	
100	Units conversion factor ([mg-m^2]/[kg-cm^2])	
Q	Source emissions (g/sec)	Waste mgt. scenario-specific
Z_{HG}	Soil mixing depth of home garden – tilled (cm)	20
BD	Soil bulk density (g/cm^3)	Site Specific
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific
0.31536	Units conversion factor (m-g-s/cm-μg-yr)	
Vdv_{HG}	Dry deposition velocity for home garden (cm/s)	0.2
Cyv_{HG}	Normalized vapor phase air concentration for home garden (μg-s/g-m^3)	Modeled ISC3
$Dywv_{HG}$	Normalized yearly wet deposition from vapor phase for home garden (s/m^2-yr)	Modeled ISC3
$Dydp_{HG}$	Normalized yearly dry deposition from particle phase for home garden (s/m^2-yr)	Modeled ISC3
$Dywp_{HG}$	Normalized yearly wet deposition from particle phase for home garden (s/m^2-yr)	Modeled ISC3

Description

This equation calculates average air deposition occurring over the exposure duration as a result of wet and dry deposition of particles onto soil, deposition of wet vapors onto soil, and diffusion of dry vapors into soil. Constituents are assumed to be incorporated only to a finite depth (the mixing depth, Z).

Table E-2.10. Aboveground Produce Concentration Due to Direct Deposition

Home Gardener Scenario

$$Pd_{HG} = \frac{1000\,x\,Q\,x\,(1 - F_v)\,x\,[Dydp_{HG} + (Fw\,x\,Dywp_{HG})]\,x\,Rp\,x\,[(1.0 - \exp(-kp\,x\,Tp)]}{Yp\,x\,kp}$$

Parameter	Definition	Central Tendency	High End
Pd_{HG}	Concentration in plant due to direct deposition (mg/kg) - Home Gardener		
1000	Units conversion factor (mg/g)		
Q	Emissions (g/s)	Waste mgt. scenario-specific	
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific	
$Dydp_{HG}$	Normalized yearly dry deposition from particle phase for home garden (s/m^2-yr)	Modeled ISC3	
Fw	Fraction of wet deposition that adheres to plant (dimensionless)	Chemical-specific	
$Dywp_{HG}$	Normalized yearly wet deposition from particle phase for home garden (s/m^2/yr)	Modeled ISC3	
Rp	Interception fraction of edible portion of plant (dimensionless)	Appendix K	
kp	Plant surface loss coefficient (1/yr)	18	
Tp	Length of plant exposure to deposition of edible portion of plant, per harvest (yrs)	Appendix K	
Yp	Yield or standing crop biomass of the edible portion of the plant (kg DW/m^2)	Appendix K	

Description

This equation calculates the constituent concentration in aboveground vegetation due to wet and dry deposition of constituent onto the plant surface.

Table E-2.11. Aboveground Produce Concentration Due to Air-to-Plant Transfer

Home Gardener Scenario

$$Pv_{HG} = Q \, x \, F_v \, x \, \frac{Cyv_{HG} \; x \; Bv \; x \; VG_{ag}}{\rho_a}$$

Parameter	Definition	Default Value
Pv_{HG}	Concentration of constituent in the plant due to air-to-plant transfer (mg/kg) - Home Gardener	
Q	Emissions (g/s)	Waste mgt. scenario-specific
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific
Cyv_{HG}	Normalized vapor phase air concentration for home garden (µg-s/g-m^3)	Modeled ISC3
Bv	Air-to-plant biotransfer factor ([mg constituent/kg plant tissue DW]/[µg constituent/g air])	Chemical-specific
VG_{ag}	Empirical correction factor for above-ground produce (dimensionless)	0.01
ρ_a	Density of air (g/cm^3)	1.2×10^{-3}

Description

This equation calculates the constituent concentration on a dry weight (DW) basis in aboveground vegetation due to direct uptake of vapor phase chemicals into the plant leaves.

Table E-2.12. Aboveground Produce Concentration Due to Root Uptake

Home Gardener Scenario

$$Pr_{HG} = C_{HG} \times Br$$

Parameter	Definition	Central Tendency	High End
Pr_{HG}	Concentration of constituent in the plant due to direct uptake from soil (mg/kg) - Home Gardener		
C_{HG}	Average soil concentration of constituent over exposure duration (mg/kg)	Calculated (see Table E-2.1.)	
Br	Plant-soil bioconcentration factor for aboveground produce [µg/g DW]/[µg/g soil]	Chemical-specific	

Description

This equation calculates the constituent concentration on a dry weight (DW) basis in aboveground vegetation due to direct uptake of chemicals from soil.

Table E-2.13. Root Vegetable Concentration Due to Root Uptake

Home Gardener Scenario

$$Pr_{bg,HG} = \frac{C_{HG}\ x\ RCF\ x\ VG_{bg}}{Kd_s}$$

Parameter	Definition	Central Tendency	High End
$Pr_{bg,\ HG}$	Concentration of constituent in belowground plant parts due to root uptake (mg/kg) - Home Gardener		
C_{HG}	Soil concentration of constituent (mg/kg)	Calculated (see Table E-2.1.)	
RCF	Ratio of concentration in roots to concentration in soil pore water ([mg constituent/kg plant tissue WW] / [μg constituent/mL pore water])	Chemical-specific	
VG_{bg}	Empirical correction factor for plant uptake - root vegetables (dimensionless)	0.01	
Kd_s	Soil-water partition coefficient (mL/g)	Metals: Chemical-specific Organics: Calculated ($Kd_s = K_{oc}$ x foc)	
K_{oc}	Octanol/water partition coefficient (mL/g)	Chemical-specific	
foc	Fraction of organic carbon in soil (dimensionless)	Site specific	

Description

This equation calculates the constituent concentration in root vegetables due to uptake from the soil water.

Table E-3.1. Constituent Concentration in Agricultural Field Due to Erosion

Farmer Exposure Scenario

$$C_{SF} = \frac{SL_{0,F} \ x \ C_0 \ x \ ER}{ks_{SF} \ x \ M_{SF}} + \frac{SL_{B,F} \ x \ C_{B/Surr} \ x \ ER}{ks_{SF} \ x \ M_{SF}} + \frac{Ds_{(1),SF}}{ks_{SF}}$$

Parameter	Definition	Central Tendency	High End
C_{SF}	Constituent concentration in agricultural field (mg/kg)		
$SL_{0,F}$	Soil load delivered to off-site location for material originating in source area (kg/yr)	Calculated (see Table E-1.2.)	
$SL_{B,F}$	Soil load delivered to off-site location for material originating in buffer area (kg/yr)	Calculated (see Table E-1.7.)	
$C_{B/Surr}$	Constituent concentration in buffer and surrounding areas (mg/kg)	Calculated (see Table E-1.11.)	
$Ds_{(1),SF}$	Deposition term for the agricultural field (mg/kg-yr)	Calculated (see Table E-3.9.)	
C_0	Source constituent concentration (mg/kg)	Chemical-specific	
ks_{SF}	Constituent loss constant from the agricultural field (1/yr)	Calculated (see Table E-3.2.)	
M_{SF}	Mass of soil in mixing depth of agricultural field (kg)	Calculated (see Table E-3.8.)	
ER	Constituent enrichment ratio (unitless)	organics = 3 metals = 1	

Description

This equation is used to calculate the mass of constituent deposited onto the agricultural field as a result of erosion from the source.

Table E-3.2. Soil Loss Constant

Farmer Exposure Scenario

$$ks_{SF} = ksl_{SF} + kse_{SF} + ksr_{SF} + ksg_{SF} + ksv_{SF}$$

Parameter	Definition	Central Tendency	High End
ks_{SF}	Constituent soil loss constant due to all processes from agricultural field (1/yr)		
ksl_{SF}	Constituent loss constant due to leaching (1/yr)	Calculated (see Table E-3.3.)	
kse_{SF}	Constituent loss constant due to soil erosion (1/yr)	Calculated (see Table E-3.4)	
ksr_{SF}	Constituent loss constant due to surface runoff (1/yr)	Calculated (see Table E-3.6.)	
ksg_{SF}	Constituent loss constant due to degradation (1/yr)	Chemical specific	
ksv_{SF}	Constituent loss constant due to volatilization (1/yr)	Calculated (see Table E-3.7.)	

Description

This equation calculates the constituent loss constant, which accounts for the loss of constituent from soil by multiple mechanisms.

Table E-3.3. Loss Constant Due to Leaching

Farmer Exposure Scenario

$$ksl_{SF} = \frac{P + I - R - E_v}{\theta \; x \; Z_{SF} \; x \; [1.0 + (BD \; x \; Kd_s / \theta)]}$$

Parameter	Definition	Central Tendency	High End
ksl_{SF}	Constituent loss constant due to leaching from an agricultural field (1/yr)		
P	Average annual precipitation (cm/yr)	Site Specific	
I	Average annual irrigation (cm/yr)	0	
R	Average annual runoff (cm/yr)	Site Specific	
E_v	Average annual evapotranspiration (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_{SF}	Soil depth of agricultural field from which leaching removal occurs – tilled (cm)	20	
BD	Soil bulk density (g/cm^3)	Site Specific	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	

Description

This equation calculates the constituent loss constant due to leaching from soil.

Table E-3.4. Constituent Loss Constant Due to Erosion

Farmer Exposure Scenario

$$kse_{SF} = \frac{0.1\ x\ ER\ x\ X_{e,SF}\ x\ [SD_{SB} + (1 - SD_{SB})(\frac{A_{BF}}{A_F\ +\ A_{BF}})]}{BD\ x\ Z_{SF}}\ x\ \left(\frac{Kd_s\ x\ BD}{\theta + (Kd_s\ x\ BD)}\right)$$

Parameter	Definition	Central Tendency	High End
kse_{SF}	Constituent loss constant due to erosion from an agricultural field (1/yr)		
$X_{e,SF}$	Unit soil loss from the agricultural field (kg/m^2-yr)	Calculated (see Table E-3.5.)	
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)	Calculated (see Table E-1.4.)	
ER	Constituent enrichment ratio (unitless)	Organics = 3 Metals = 1	
BD	Soil bulk density (g/cm^3)	Site Specific	
Z_{SF}	Soil mixing depth of agricultural field–tilled (cm)	20	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
A_F	Area of agricultural field (m^2)	2,000,000	
A_{BF}	Area of buffer between agricultural field and waterbody (m^2)	Calculated (see Table E-1.29.)	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-3.5. Universal Soil Loss Equation (USLE) for Agricultural Field

Farmer Exposure Scenario

$$X_{e,SF} = RF_{SF} \times K_{SF} \times LS_{SF} \times C_{SF} \times P_{SF} \times \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,SF}$	Unit soil loss from the agricultural field (kg/m^2-yr)		
RF_{SF}	USLE rainfall factor (1/yr)	Site Specific	
K_{SF}	USLE erodibility factor (ton/acre)	Site Specific	
LS_{SF}	USLE length-slope factor (unitless)	Site Specific	
C_{SF}	USLE cover management factor (unitless)	Site Specific	
P_{SF}	USLE erosion control practice factor (unitless)	Site Specific	
907.18	Conversion factor (kg/ton)		
4047	Conversion factor (m^2/acre)		

Description

This equation is used to calculate the soil loss rate from the agricultural field using the Universal Soil Loss Equation.

Table E-3.6. Constituent Loss Constant Due to Runoff

Farmer Exposure Scenario

$$ksr_{SF} = \frac{R}{\theta \, x \, Z_{SF}} \, x \left(\frac{1}{1 + (Kd_s \, x \, BD/\theta)} \right)$$

Parameter	Definition	Central Tendency	High End
ksr_{SF}	Constituent loss constant due to runoff from agricultural field (1/yr)		
R	Average annual runoff (cm/yr)	Site Specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_{SF}	Soil mixing depth of tilled agricultural field (cm)	20	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
BD	Soil bulk density (g/cm^3)	Site Specific	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-3.7. Constituent Loss Constant Due to Volatilization

Farmer Exposure Scenario

$$ksv_{SF} = \left[\frac{3.1536x10^{7} \, x \, H}{Z_{SF} \, x \, Kd_{s} \, x \, R \, x \, T \, x \, BD}\right] x \left[0.482 \, x \, u^{0.78} \, x \left(\frac{\mu_a}{\rho_a \, x \, D_a}\right)^{-0.67} x \left(\sqrt{\frac{4 \, x \, A_F}{\pi}}\right)^{-0.11}\right]$$

Parameter	Definition	Central Tendency	High End
ksv_{SF}	Constituent loss constant due to volatilization for agricultural field (1/yr)		
$3.1536x10^{7}$	Conversion constant (s/yr)		
H	Henry's law constant (atm-m^3/mol)	Chemical-specific	
Z_{SF}	Soil mixing depth of tilled agricultural field (cm)	20	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
R	Universal gas constant (atm-m^3/mol-K)	$8.205x10^{-5}$	
T	Ambient air temperature (K)	Site Specific	
BD	Soil bulk density (g/cm^3)	Site Specific	
u	Average annual windspeed (m/s)	Site Specific	
μ_a	Viscosity of air (g/cm-s)	$1.81x10^{-4}$	
ρ_a	Density of air (g/cm^3)	$1.2x10^{-3}$	
D_a	Diffusivity of constituent in air (cm^2/s)	Chemical-specific	
A_F	Area of agricultural field (m^2)	2,000,000	

Description

This equation calculates the constituent loss constant due to volatilization from soil.

Table E-3.8. Mass of Soil in Mixing Depth of Agricultural Field

Farmer Exposure Scenario

$$M_{SF} = Z_{SF} \ x \ A_F \ x \ BD \ x \ 10$$

Parameter	Definition	Central Tendency	High End
M_{SF}	Mass of soil in mixing depth of agricultural field (kg)		
Z_{SF}	Soil mixing depth for tilled agricultural field (cm)	20	
A_F	Area of agricultural field (m^2)	2,000,000	
BD	Soil bulk density (g/cm^3)	Site Specific	
10	Units conversion factor		

Description

This equation is used to calculate the total mass of soil in the agricultural field that will be mixed with the mass of eroded material.

Table E-3.9. Deposition Rate Factor to Agricultural Field from Source

Farmer Exposure Scenario

$$Ds_{(1),SF} = \frac{100 \, x \, Q}{Z_{SF} \, x \, BD} \, x \, [F_v \, (0.31536 \, x \, Vdv_{SF} \, x \, Cyv_{SF} + Dywv_{SF}) + (Dydp_{SF} + Dywp_{SF}) \, x \, (1 - F_v)]$$

Parameter	Definition	Input Value
$Ds_{(1),SF}$	Deposition term for agricultural field (mg/kg-yr)	
100	Units conversion factor ([mg-m^2]/[kg-cm^2])	
Q	Source emissions (g/sec)	Waste mgt. scenario-specific
Z_{SF}	Soil mixing depth of tilled agricultural field (cm)	20
BD	Soil bulk density (g/cm^3)	Site Specific
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific
0.31536	Units conversion factor (m-g-s/cm-μg-yr)	
Vdv_{SF}	Dry deposition velocity for agricultural field (cm/s)	0.2
Cyv_{SF}	Normalized vapor phase air concentration for agricultural field (μg-s/g-m^3)	Modeled ISC3
$Dywv_{SF}$	Normalized yearly wet deposition from vapor phase for agricultural field (s/m^2-yr)	Modeled ISC3
$Dydp_{SF}$	Normalized yearly dry deposition from particle phase for agricultural field (s/m^2-yr)	Modeled ISC3
$Dywp_{SF}$	Normalized yearly wet deposition from particle phase for agricultural field (s/m^2-yr)	Modeled ISC3

Description

This equation calculates average air deposition occurring over the exposure duration as a result of wet and dry deposition of particles onto soil, deposition of wet vapors into soil, and diffusion of dry vapors into soil. Constituents are assumed to be incorporated only to a finite depth (the mixing depth, Z).

Table E-3.10. Aboveground Produce Concentration Due to Direct Deposition

Farmer Exposure Scenario

$$Pd_{SF} = \frac{1000 \, x \, Q \, x \, (1 - F_v) \, x \, [Dydp_{SF} + (Fw \, x \, Dywp_{SF})] \, x \, Rp \, x \, [(1.0 - \exp(-kp \, x \, Tp)]}{Yp \, x \, kp}$$

Parameter	Definition	Central Tendency	High End
Pd_{SF}	Concentration in plant due to direct deposition (mg/kg) - Farmer		
1000	Units conversion factor (mg/g)		
Q	Emissions (g/s)	Waste mgt. scenario-specific	
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific	
$Dydp_{SF}$	Normalized yearly dry deposition from particle phase (s/m^2-yr)	Modeled ISC3	
Fw	Fraction of wet deposition (particles) that adheres to plant (dimensionless)	Chemical-specific	
$Dywp_{SF}$	Normalized yearly wet deposition from particle phase for agricultural field (s/m^2-yr)	Modeled ISC3	
Rp	Interception fraction of edible portion of plant (dimensionless)	Appendix K	
kp	Plant surface loss coefficient (1/yr)	Appendix K	
Tp	Length of plant exposure to deposition of edible portion of plant, per harvest (yrs)	Appendix K	
Yp	Yield or standing crop biomass of the edible portion of the plant (kg DW/m^2)	Appendix K	

Description

This equation calculates the constituent concentration in aboveground vegetation due to wet and dry deposition of constituents adsorbed to particles onto the plant surface.

Table E-3.11. Aboveground Produce Concentration Due to Air-to-Plant Transfer

Farmer Exposure Scenario

$$Pv_{SF} = Q \, x \, F_v \, x \, \frac{Cyv_{SF} \, x \, Bv \, x \, VG_{ag}}{\rho_a}$$

Parameter	Definition	Default Value
Pv_{SF}	Concentration of constituent in the plant due to air-to-plant transfer (mg/kg) - Farmer	
Q	Emissions (g/s)	Waste mgt. scenario-specific
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific
Cyv_{SF}	Normalized vapor phase air concentration for agricultural field (µg-sec/g-m^3)	Modeled ISC3
Bv	Air-to-plant biotransfer factor ([mg constituent/kg plant tissue DW]/[µg constituent/g air])	Chemical-specific
VG_{ag}	Empirical correction factor for above-ground produce (dimensionless)	0.01
ρ_a	Density of air (g/cm^3)	1.2×10^{-3}

Description

This equation calculates the constituent concentration in aboveground vegetation due to direct uptake of vapor phase chemical into the plant leaves.

Table E-3.12. Aboveground Produce Concentration Due to Root Uptake

Farmer Exposure Scenario

$$Pr_{SF} = C_{SF} \times Br$$

Parameter	Definition	Central Tendency	High End
Pr_{SF}	Concentration of constituent in the plant due to direct uptake from soil (mg/kg) - Farmer		
C_{SF}	Soil concentration of constituent (mg/kg)	Calculated (see Table E-3.1.)	
Br	Plant-soil bioconcentration factor for aboveground produce [µg/g DW]/[µg/g soil]	Chemical-specific	

Description

This equation calculates the constituent concentration in aboveground vegetation due to direct uptake of chemicals from soil.

Table E-3.13. Root Vegetable Concentration Due to Root Uptake

Farmer Exposure Scenario

$$Pr_{bg,SF} = \frac{C_{SF}\ x\ RCF\ x\ VG_{bg}}{Kd_s}$$

Parameter	Definition	Central Tendency	High End
$Pr_{bg,\ SF}$	Concentration of constituent in belowground plant parts due to root uptake (mg/kg) - Farmer		
C_{SF}	Soil concentration of constituent (mg/kg)	Calculated (see Table E-3.1.)	
RCF	Ratio of concentration in roots to concentration in soil pore water ([mg constituent/kg plant tissue WW] / [μg constituent/mL pore water])	Chemical-specific	
VG_{bg}	Empirical correction factor for plant uptake - root vegetables (dimensionless)	0.01	
Kd_s	Soil-water partition coefficient (mL/g)	Metals: Chemical-specific Organics: Calculated ($Kd_s = K_{oc}$ x foc)	
K_{oc}	Octanol/water partition coefficient (mL/g)	Chemical-specific	
foc	Fraction of organic carbon in soil (dimensionless)	Site specific	

Description

This equation calculates the constituent concentration in root vegetables due to uptake from the soil water.

Table E-3.14. Beef Concentration Due to Plant and Soil Ingestion

Farmer Scenario

$$A_{beef} = (F\ x\ Qp\ x\ P + Qs\ x\ C_{SF})\ x\ Ba_{beef}$$

Parameter	Definition	Central Tendency	High End
A_{beef}	Concentration of constituent in beef (mg/kg)		
F	Fraction of plant grown on contaminated soil and eaten by the animal- grain or forage (dimensionless)	1	
Qp	Quantity of plant eaten by the animal each day (kg plant tissue DW/day) - beef cattle–grain - beef cattle–forage	Appendix K	
P	Total concentration of constituent in the plant eaten by the animal (mg/kg) = Pd + Pv + Pr	Calculated (see Tables E-3.16, E-3.17, E-3.18)	
Qs	Quantity of soil eaten by the foraging animal (kg soil/day)	Appendix K	
C_{SF}	Soil concentration in agricultural field (mg/kg)	Calculated (see Table E-3.1)	
Ba_{beef}	Biotransfer factor for beef (d/kg)	Chemical-specific	

Description

This equation calculates the concentration of constituent in beef from ingestion of forage and soil.

Table E-3.15. Milk Concentration Due to Plant and Soil Ingestion

Farmer Scenario

$$A_{milk} = (F \times Qp \times P + Qs \times C_{SF}) \times Ba_{milk}$$

Parameter	Definition	Central Tendency	High End
A_{milk}	Concentration of constituent in milk (mg/kg)		
F	Fraction of plant grown on contaminated soil and eaten by the animal - grain or forage (dimensionless)	1	
Qp	Quantity of plant eaten by the animal each day (kg plant tissue DW/day) - dairy cattle–grain - dairy cattle–forage	Appendix K	
P	Total concentration of constituent in the plant eaten by the animal (mg/kg) = Pd + Pv + Pr	Calculated (see Tables E-3.16., E-3.17., E-3.18.)	
Qs	Quantity of soil eaten by the foraging animal (kg soil/day)	Appendix K	
C_{SF}	Soil concentration (mg/kg)	Calculated (see Table E-3.1.)	
Ba_{milk}	Biotransfer factor for milk (day/kg)	Chemical-specific	

Description

This equation calculates the concentration of constituent in milk from ingestion of forage and soil.

Table E-3.16. Forage (Pasture Grass/Hay) Concentration Due to Direct Deposition

Farmer Scenario

$$Pd = \frac{1000\,x\,Q\,x\,(1 - F_v)[Dydp_{SF} + (Fw\,x\,Dywp_{SF})]\,x\,Rp\,x\,[(1.0 - \exp(-kp\,x\,Tp))]}{Yp\,x\,kp}$$

Parameter	Definition	Central Tendency	High End
Pd	Concentration in plant due to direct deposition (mg/kg)		
1000	Units conversion factor (mg/g)		
Q	Emissions (g/s)	Waste mgt. scenario-specific	
F_v	Fraction of constituent concentration present in the vapor phase (dimensionless)	Chemical-specific	
$Dydp_{SF}$	Normalized yearly dry deposition from particle phase (s/m^2-yr)	Modeled ISC3	
Fw	Fraction of wet deposition (particles) that adheres to plant surfaces (dimensionless)	Chemical-specific	
$Dywp_{SF}$	Normalized yearly wet deposition from particle phase for agricultural field (s/m^2-yr)	Modeled ISC3	
Rp	Interception fraction of edible portion of plant (dimensionless)	Appendix K	
kp	Plant surface loss coefficient (1/yr)	18	
Tp	Length of the plant exposure to deposition onto edible portion of plant per harvest (yrs)	Appendix K	
Yp	Yield or standing crop biomass of the edible portion of the plant (kg DW/m^2)	Appendix K	

Description

This equation calculates the constituent concentration in aboveground vegetation due to wet and dry deposition of constituents adsorbed to particles onto the plant surface.

Table E-3.17. Forage (Pasture Grass/Hay) Concentration Due to Air-to-Plant Transfer

Farmer Scenario

$$Pv = \frac{Cv_{SF} \ x \ Bv \ x \ VG_{ag}}{\rho_a}$$

Parameter	Definition	Central Tendency	High End
Pv	Concentration of constituent in the plant due to air-to-plant transfer (mg/kg)		
Cv_{SF}	Vapor phase air concentration of constituent in air due to direct emissions (μg constituent/m^3)	Modeled ISC3	
Bv	Air-to-plant biotransfer factor ([mg constituent/kg plant tissue DW]/[μg [constituent/g air])	Chemical-specific	
VG_{ag}	Empirical correction factor that reduces produce concentration because Bv was developed for azalea leaves.	1.0	
ρ_a	Density of air (g/cm^3)	1.2×10^{-3}	

Description

This equation calculates the constituent concentration in aboveground vegetation due to direct uptake of vapor phase chemicals into the plant leaves.

Table E-3.18. Forage/Silage/Grain Concentration Due to Root Uptake

Farmer Scenario

$$Pr = \sum_i C_{SF} \times Br_i$$

Parameter	Definition	Default Value
Pr	Concentration of constituent in the plant due to direct uptake from soil (mg/kg)	
C_{SF}	Average soil concentration of constituent over exposure duration (mg/kg)	Calculated (see Table E-3.1.)
Br_i	Plant-soil bioconcentration factor for plant species i (forage/silage/grain) [μg/g DW]/[μg/g soil]	Chemical-specific

Description

This equation calculates the constituent concentration in aboveground vegetation due to direct uptake of constituents from soil.

Table E-4.1. Watershed Constituent Concentration

All Exposure Scenarios

$$C_{WS} = \frac{Ds_{(1)WS}}{ks_{ws}}$$

Parameter	Definition	Central Tendency	High End
C_{WS}	Constituent concentration in watershed area outside of sub-basin (mg/kg)		
$Ds_{(1),WS}$	Deposition term for the watershed (mg/kg-yr)	Calculated (see Table E-4.2.)	
ks_{WS}	Constituent loss constant from the watershed (1/yr)	Calculated (see Table E-4.3.)	

Description

This equation is used to calculate the mass of constituent deposited onto the watershed area outside of sub-basin as a result of air deposition.

Table E-4.2. Deposition Rate Factor to Watershed from Source

All Exposure Scenarios

$$Ds_{(1)WS} = \frac{100 x Q}{Z_{WS} x BD} \; [F_v \; (0.31536 \; x \; Vdv_{WS} \; x \; Cyv_{WS} + Dywv_{WS}) + (Dydp_{WS} + Dywp_{WS}) \; x \; (1 - F_v)]$$

Parameter	Definition	Central Tendency	High End
$Ds_{(1)WS}$	Deposition rate factor for the watershed (mg/kg-yr)		
100	Units conversion factor ([mg-m^2]/[kg-cm^2])		
Q	Source emissions (g/s)	Waste management scenario specific	
Z_{WS}	Soil mixing depth in watershed area (cm)	2.5	
BD	Soil bulk density (g/cm^3)	Site specific	
F_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific	
0.31536	Units conversion factor (mg-g-s/cm-µg-yr)		
Vdv_{WS}	Dry deposition velocity of vapors to watershed (cm/s)	0.2	
Cyv_{WS}	Normalized vapor phase air concentration for watershed (µg-s/g-m^3)	Modeled ISC3	
$Dywv_{WS}$	Normalized yearly wet deposition from vapor phase for watershed (s/m^2-yr)	Modeled ISC3	
$Dydp_{WS}$	Normalized yearly dry deposition from particle phase for watershed (s/m^2-yr)	Modeled ISC3	
$Dywp_{WS}$	Normalized yearly wet deposition from particle phase for watershed (s/m^2-yr)	Modeled ISC3	

Description

This equation calculates average air deposition occurring over the exposure duration as a result of wet and dry deposition of particles onto soil, deposition of wet vapors onto soil, and diffusion of dry vapors into soil. Constituents are assumed to be incorporated only to a finite depth (the mixing depth, Z).

Table E-4.3. Constituent Loss Constant

All Exposure Scenarios

$$ks_{WS} = ksl_{WS} + kse_{WS} + ksr_{WS} + ksg_{WS} + ksv_{WS}$$

Parameter	Definition	Central Tendency	High End
ks_{WS}	Constituent loss constant due to all processes from watershed (1/yr)		
ksl_{WS}	Constituent loss constant for watershed due to leaching (1/yr)	Calculated (see Table E-4.4.)	
kse_{WS}	Constituent loss constant for watershed due to soil erosion (1/yr)	Calculated (see Table E-4.5.)	
ksr_{WS}	Constituent loss constant for watershed due to surface runoff (1/yr)	Calculated (see Table E-4.8.)	
ksg_{WS}	Constituent loss constant for watershed due to degradation (1/yr)	Chemical specific	
ksv_{WS}	Constituent constant for watershed due to volatilization (1/yr)	Calculated (see Table E-4.9.)	

Description

This equation calculates the constituent loss constant, which accounts for the loss of constituent from soil by multiple mechanisms.

Table E-4.4. Constituent Loss Constant Due to Leaching

All Exposure Scenarios

$$ksl_{WS} = \frac{P + I - R - E_v}{\theta \; x \; Z_{WS} \; x \; [1.0 + (BD \; x \; Kd_s / \theta)]}$$

Parameter	Definition	Central Tendency	High End
ksl_{WS}	Constituent loss constant for watershed due to leaching (1/yr)		
P	Average annual precipitation (cm/yr)	Site specific	
I	Average annual irrigation (cm/yr)	0	
R	Average annual runoff (cm/yr)	Site specific	
E_v	Average annual evapotranspiration (cm/yr)	Site specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_{WS}	Soil depth for watershed from which leaching removal occurs – untilled (cm)	2.5	
BD	Soil bulk density (g/cm^3)	Site specific	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical specific	

Description

This equation calculates the constituent loss constant due to leaching from soil.

Table E-4.5. Constituent Loss Constant Due to Erosion

All Exposure Scenarios

$$kse_{WS} = \frac{0.1\ x\ X_{e,WS}\ x\ SD_{WS}\ x\ ER}{BD\ x\ Z_{WS}}\ x \left(\frac{Kd_s\ x\ BD}{\theta + (Kd_s\ x\ BD)} \right)$$

Parameter	Definition	Central Tendency	High End
kse_{WS}	Constituent loss constant due to erosion for watershed (1/yr)		
$X_{e,WS}$	Unit soil loss for watershed (kg/m^2-yr)	Calculated (see Table E-4.6.)	
SD_{WS}	Sediment delivery ratio for watershed (unitless)	Calculated (see Table E-4.7.)	
ER	Constituent enrichment ratio (unitless)	Organics = 3 Metals = 1	
BD	Soil bulk density (g/cm^3)	Site specific	
Z_{WS}	Soil mixing depth in watershed – untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
0.1	Units conversion factor (g-m^2)/(kg-cm^2)		

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-4.6. Universal Soil Loss Equation (USLE) for the Watershed

All Exposure Scenarios

$$X_{e,WS} = R_{WS} \ x \ K_{WS} \ x \ LS_{WS} \ x \ C_{WS} \ x \ P_{WS} \ x \ \frac{907.18}{4047}$$

Parameter	Definition	Central Tendency	High End
$X_{e,WS}$	Unit soil loss from the watershed (kg/m^2 -yr)		
R_{WS}	USLE rainfall factor (1/yr)	Site specific	
K_{WS}	USLE erodibility factor (ton/acre)	Site specific	
LS_{WS}	USLE length-slope factor (unitless)	Site specific	
C_{WS}	USLE cover factor (unitless)	Site specific	
P_{WS}	USLE erosion control practice factor (unitless)	Site specific	
907.18	Units conversion factor (kg/ton)		
4047	Units conversion factor (m^2/acre)		

Description

This equation is used to calculate the soil loss rate from the watershed using the Universal Soil Loss Equation.

Table E-4.7. Sediment Delivery Ratio

Fisher Scenario

$$SD_{WS} = a \ x \ (A_{WS})^{-b}$$

Parameter	**Definition**	**Central Tendency**	**High End**
SD_{WS}	Sediment delivery ratio for watershed (unitless)		
a	Empirical intercept coefficient	Depends on watershed area; see table below	
A_{WS}	Area of watershed area receiving fallout (m^2)	NA	
b	Empirical slope coefficient	0.125	

Description

This equation calculates the sediment delivery ratio for the watershed.

Values for Empirical Intercept Coefficient, a

Watershed area (sq. miles)	"a" coefficient (unitless)
$\leq$ 0.1	2.1
1	1.9
10	1.4
100	1.2
1,000	0.6
1 sq. mile = 2.59×10^6 m^2	

Table E-4.8. Constituent Loss Constant Due to Runoff

All Exposure Scenarios

$$ksr_{WS} = \frac{R}{\theta \ x \ Z_{WS}} \ x \ \left(\frac{1}{1 + (Kd_s \ x \ BD/\theta)}\right)$$

Parameter	Definition	Central Tendency	High End
ksr_{WS}	Constituent loss constant due to runoff for watershed (1/yr)		
R	Average annual runoff (cm/yr)	Site specific	
θ	Soil volumetric water content (mL/cm^3)	Calculated (see Table E-1.17.)	
Z_{WS}	Soil mixing depth in watershed – untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical-specific	
BD	Soil bulk density (g/cm^3)	Site specific	

Description

This equation calculates the constituent loss constant due to runoff from soil.

Table E-4.9. Constituent Loss Constant Due to Volatilization

All Exposure Scenarios

$$ksv_{WS} = \left[\frac{3.1536x10^{7}\,x\,H}{Z_{WS}\,x\,Kd_{s}\,x\,R\,x\,T\,x\,BD}\right] x \left[0.482\,x\,u^{0.78}\,x\left(\frac{\mu_a}{\rho_a\,x\,D_a}\right)^{-0.67} x\left(\sqrt{\frac{4\,x\,A_{WS}}{\pi}}\right)^{-0.11}\right]$$

Parameter	Definition	Central Tendency	High End
ksv_{WS}	Constituent loss constant due to volatilization for watershed (1/yr)		
$3.1536x10^7$	Conversion constant (s/yr)		
H	Henry's law constant (atm-m^3/mol)	Chemical specific	
Z_{WS}	Soil mixing depth in watershed – untilled (cm)	2.5	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical specific	
R	Universal gas constant (atm-m^3/mol-K)	$8.205x10^{-5}$	
T	Ambient air temperature (K)	Site specific	
BD	Soil bulk density (g/cm^3)	Site specific	
u	Average annual windspeed (m/s)	Site specific	
μ_a	Viscosity of air (g/cm-s)	$1.81x10^{-4}$	
ρ_a	Density of air (g/cm^3)	$1.2x10^{-3}$	
D_a	Diffusivity of constituent in air (cm^2/s)	Chemical specific	
A_{WS}	Total watershed surface area (m^2)	NA	

Description

This equation calculates the constituent loss constant due to volatilization from soil.

Table E-4.10. Total Waterbody Load

Fisher Scenario			
$$L_T = L_{Dep} + L_{Dif} + L_{RI} + L_R + L_E$$			
Parameter	**Definition**	**Central Tendency**	**High End**
L_T	Total constituent load to the waterbody (g/yr)		
L_{Dep}	Total (wet and dry) particle phase and wet vapor phase direct deposition load to waterbody (g/yr)	Calculated (see Table E-4.11.)	
L_{Dif}	Vapor phase constituent diffusion load to waterbody (g/yr)	Calculated (see Table E-4.12.)	
L_{RI}	Runoff load from impervious surfaces (g/yr)	Calculated (see Table E-4.16.)	
L_R	Runoff load from pervious surfaces (g/yr)	Calculated (see Table E-4.17.)	
L_E	Soil erosion load (g/yr)	Calculated (see Table E-4.19.)	
Description			
This equation calculates the total average waterbody load from wet and dry vapor and particle deposition, runoff, and erosion loads.			

Table E-4.11. Deposition to Waterbody

Fisher Scenario

$$L_{Dep} = Q \; x \; [\, f_v \; x \; Dywv + (\, 1 - f_v \,) \; x \; Dytwp] \; x \; WA_w$$

Parameter	Definition	Central Tendency	High End
L_{Dep}	Total (wet and dry) particle phase and wet vapor phase direct deposition load to waterbody (g/yr)		
Q	Source emissions (g/s)	Waste management scenario-specific	
f_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific	
Dywv	Normalized yearly average wet deposition from vapor phase for the waterbody (s/m^2-yr)	Modeled ISC3	
Dytwp	Normalized yearly average wet and dry deposition from particle phase for the waterbody (s/m^2-yr)	Modeled ISC3	
WA_w	Area of waterbody area (m^2)	Site specific	

Description

This equation calculates the average load to the waterbody from direct wet and dry deposition of particles and wet deposition of vapors onto the surface of the waterbody.

Table E-4.12. Diffusion Load to Waterbody

Fisher Scenario

$$L_{Dif} = \frac{K_v \; x \; Q \; x \; f_v \; x \; Cywv \; x \; WA_w \; x \; 10^{-6}}{\dfrac{H}{R \; x \; T_w}}$$

Parameter	Definition	Central Tendency	High End
L_{Dif}	Dry vapor phase constituent diffusion load to waterbody (g/yr)		
K_v	Diffusive mass transfer coefficient (m/yr)	Calculated (see Table E-4.13.)	
Q	Source emissions (g/s)	Waste management scenario specific	
f_v	Fraction of air concentration in vapor phase (dimensionless)	Chemical-specific	
Cywv	Normalized average vapor phase air concentration for waterbody (μg-s/g-m^3)	Modeled ISC3	
WA_w	Waterbody surface area (m^2)	Site specific	
10^{-6}	Units conversion factor (g/µg)		
H	Henry's law constant (atm-m^3/mol)	Chemical specific	
R	Universal gas constant (atm-m^3/mol-K)	$8.205 x 10^{-5}$	
T_w	Waterbody temperature (K)	298	

Description

This equation calculates the load to the waterbody due to vapor diffusion.

Table E-4.13. Overall Transfer Rate

Fisher Scenario

$$K_v = \left[K_L^{-1} + \left(K_G \frac{H}{R \ x \ T_k} \right)^{-1} \right]^{-1} x \ \theta^{(T_k - 293)}$$

Parameter	Definition	Central Tendency	High End
K_v	Overall transfer rate (m/yr)		
K_L	Liquid phase transfer coefficient (m/yr)	Calculated (see Table E-4.14.)	
K_G	Gas phase transfer coefficient (m/yr)	Calculated (see Table E-4.15.)	
H	Henry's Law constant (atm-m^3/mol)	Chemical specific	
R	Universal gas constant (atm-m^3/mol-K)	8.205×10^{-5}	
T_k	Waterbody temperature (K)	298	
θ	Temperature correction factor (unitless)	1.026	

Description

This equation calculates the overall transfer rate of constituent from the liquid and gas phases in surface water.

Table E-4.14. Liquid Phase Transfer Coefficient

Fisher Scenario

- Flowing stream or river

$$K_L = \sqrt{\frac{10^{-4} \ x \ D_w \ x \ u}{d_z}} \ x \ 3.15 \ x \ 10^7$$

- Quiescent lake or pond

$$K_L = (C_d^{0.5} \ x \ W) \ x \left(\frac{\rho_a}{\rho_w}\right)^{0.5} x \left(\frac{k^{0.33}}{\lambda_2}\right) x \left(\frac{\mu_w}{\rho_w \ x \ D_w}\right)^{-0.67} x \ 3.15 x 10^7$$

$$\rho_w = 1 - 8.8 \ x \ 10^{-5} \ x \ (T_k - 273)$$

Parameter	Definition	Central Tendency	High End
K_L	Liquid phase transfer coefficient (m/yr)		
D_w	Diffusivity of chemical in water (cm^2/s)	Chemical specific	
u	Current velocity (m/s)	Site specific	
d_z	Total waterbody depth (m)	Calculated (d_w+d_b)	
C_d	Drag coefficient (unitless)	0.0011	
W	Wind velocity, 10 m above water surface (m/s)	Site specific	
ρ_a	Density of air corresponding to water temperature (g/cm^3)	1.2 x 10^{-3}	
ρ_w	Density of water corresponding to water temperature (g/cm^3)	Calculated	
k	von Karman's constant (unitless)	0.4	
λ_2	Dimensionless viscous sublayer thickness	4	
μ_w	Viscosity of water corresponding to the water temperature (g/cm-s)	1.69 x 10^{-2}	
3.15x10^7	Conversion constant (s/yr)		
10^{-4}	Units conversion factor (m^2/cm^2)		
T_K	Waterbody temperature (K)	298	

Description

This equation calculates the transfer rate of constituent from the liquid phase for a flowing or quiescent system.

Table E-4.15. Gas Phase Transfer Coefficient

Fisher Scenario

- Flowing stream or river

$$K_G = 36500 m/yr$$

- Quiescent lake or pond

$$K_G = (C_d^{0.5} \ x \ W) \ x \left(\frac{k^{0.33}}{\lambda_2} \right) \ x \left(\frac{\mu_a}{\rho_a \ x \ D_a} \right)^{-0.67} \ x \ 3.15x10^7$$

Parameter	Definition	Central Tendency	High End
K_G	Gas phase transfer coefficient (m/yr)		
C_d	Drag coefficient (unitless)	0.0011	
W	Wind velocity, 10 m above water surface (m/s)	Site specific	
k	von Karman's constant (unitless)	0.4	
λ_2	Dimensionless viscous sublayer thickness (unitless)	4	
μ_a	Viscosity of air corresponding to the air temperature (g/cm-s)	1.81×10^{-4}	
ρ_a	Density of air corresponding to water temperature (g/cm^3)	1.2×10^{-3}	
D_a	Diffusivity of chemical in air (cm^2/s)	Chemical specific	
$3.15x10^7$	Conversion constant (s/yr)		

Description

This equation calculates the transfer rate of constituent from the gas phase for a flowing or quiescent system.

Table E-4.16. Impervious Runoff Load to Waterbody

Fisher Scenario

$$L_{RI} = Q\ x\ [\,f_v\ x\ Dywv + (\,1.0 - f_v\,)\ x\ Dytwp]\ x\ A_I$$

Parameter	Definition	Central Tendency	High End
L_{RI}	Impervious surface runoff load (g/yr)		
A_I	Impervious watershed area receiving pollutant deposition (m^2)	2.05×10^9	
Q	Source emissions (g/s)	Waste mgt. scenario specific	
f_v	Fraction of constituent concentration in vapor phase (dimensionless)	Chemical-specific	
Dywv	Normalized yearly watershed average wet deposition from vapor phase (s/m^2-yr)	Modeled ISC3	
Dytwp	Normalized yearly watershed average total (wet and dry) deposition from particle phase (s/m^2-yr)	Modeled ISC3	

Description

This equation calculates the average runoff load to the waterbody from impervious surfaces in the watershed from which runoff is conveyed directly to the waterbody.

Table E-4.17. Pervious Runoff Load to Waterbody

Fisher Scenario

$$L_R = R \; x \; (A_{WS} - A_I) \; x \; \frac{S_C \; x \; BD}{\theta + Kd_s \; x \; BD} \; x \; 0.01$$

Parameter	Definition	Central Tendency	High End
L_R	Pervious surface runoff load (g/yr)		
R	Average annual surface runoff (cm/yr)	Site specific	
S_c	Weighted average constituent concentration in total watershed soils (watershed and sub-basin) based on surface area (mg/kg)	Calculated (see Table E-4.18.)	
BD	Soil bulk density (g/cm^3)	Site specific	
Kd_s	Soil-water partition coefficient cm^3/g)	Chemical specific	
A_{WS}	Total watershed area (m^2)	NA	
A_I	Impervious watershed area receiving constituent deposition (m^2)	2.05×10^9	
0.01	Units conversion factor (kg-cm^2/mg-m^2)		
θ	Volumetric soil water content (ml/cm^3)	Calculated (see Table E-1.17.)	

Description

This equation calculates the average runoff load to the waterbody from pervious soil surfaces in the watershed.

Table E-4.18. Constituent Concentration in Total Watershed Soils Based on Surface Area

All Exposure Scenarios

$$S_C = \frac{A_S\, x\, C_0 + A_F\, x\, C_R + A_{B/Surr}\, x\, C_{B/Surr} + (A_{WS} - A_S - A_{B/Surr} - A_F)\, x\, C_{WS}}{A_{WS}}$$

Parameter	Definition	Central Tendency	High End
S_C	Weighted average constituent concentration in total watershed soils (watershed and sub-basin soils) based on surface area (mg/kg)		
A_S	Area of source (m^2)	Waste management scenario specific	
C_0	Source constituent concentration (mg/kg)	Chemical specific	
A_F	Area of residential plot (m^2)	5,100	
C_R	Constituent concentration in residential plot - Adult resident (mg/kg)	Calculated (see Table E-1.1.)	
$A_{B/Surr}$	Area of buffer and surrounding areas (m^2)	Calculated (see Table E-1.5.)	
$C_{B/Surr}$	Constituent concentrations in buffer and surrounding area (mg/kg)	Calculated (see Table E-1.11.)	
A_{WS}	Area of entire watershed (m^2)	NA	
C_{WS}	Constituent concentrations in watershed (mg/kg)	Calculated (see Table E-4.1.)	

Description

This equation is used to calculate the weighted average constituent concentration in the total watershed soils, using the constituent concentration in the watershed soils and the constituent concentration in each of the areas within the sub-basin (e.g., source, residential plot, and buffer and surrounding area).

Table E-4.19. Erosion Load to Waterbody

Fisher Scenario

$$L_E = X_{e,ws} \ x \ (A_{WS} - A_I) \ x \ SD_{WS} \ x \ ER \ x \ \frac{S_{c,soil} \ x \ Kd_s \ x \ BD}{\theta + Kd_s \ x \ BD} \ x \ 0.001$$

Parameter	Definition	Central Tendency	High End
L_E	Constituent load via soil erosion (g/yr)		
$X_{e,WS}$	Unit soil loss from the watershed (kg/m^2-yr)	Calculated (see Table E-4.6)	
$S_{c,soil}$	Weighted average total watershed soil (watershed and sub-basin) concentration based on sediment transport (mg/kg)	Calculated (see Table E-4.20.)	
BD	Soil bulk density (g/cm^3)	Site specific	
θ	Volumetric soil water content (ml/cm^3)	Calculated (see Table E-1.17)	
Kd_s	Soil-water partition coefficient (cm^3/g)	Chemical specific	
A_{WS}	Total watershed area (m^2)	NA	
A_I	Impervious watershed area (m^2)	2.05×10^9	
SD_{WS}	Sediment delivery ratio for watershed (unitless)	Calculated (see Table E-4.7.)	
ER	Soil enrichment ratio (unitless)	Organics = 3 Metals = 1	
0.001	Units conversion factor (g/mg)		

Description

This equation calculates the load to the waterbody from soil erosion.

Table E-4.20. Weighted Average Soil Concentration Based on Eroded Soil Contributions

All Exposure Scenarios

$$S_{c,soil} = \left[\frac{(X_{e,S}\ x\ A_S\ x\ C_0\ x\ SD_{SB}) + (X_{e,B/Surr}\ x\ A_{B/Surr}\ x\ C_{B/Surr}\ x\ SD_{SB}) + (X_{e,R}\ x\ A_F\ x\ C_R\ x\ SD_{SB})}{X_{e,WS}\ x\ A_{WS}\ x\ SD_{WS}} \right]$$

$$+ \frac{(A_{ws} - A_s - A_{B/Surr} - A_F)\ x\ C_{ws}}{A_{ws}}$$

Parameter	Definition	Input Value
$S_{c,\ soil}$	Weighted average total watershed soil (watershed and sub-basin) concentration based on eroded soil (mg/kg)	
$X_{e,S}$	Unit soil loss from source (kg/m^2-yr)	Calculated (see Table E-1.3.)
A_S	Source area (m^2)	Waste management scenario specific
C_0	Source constituent concentration (mg/kg)	Constituent specific
SD_{SB}	Sediment delivery ratio for sub-basin (unitless)	Calculated (see Table E-1.4.)
$X_{e,B/Surr}$	Unit soil loss from buffer and surrounding areas (kg/m^2-yr)	Calculated (see Table E-1.20.)
$A_{B/Surr}$	Buffer and surrounding areas (m^2)	Calculated (see Table E-1.5.)
$C_{B/Surr}$	Buffer and surrounding areas constituent concentration (mg/kg)	Calculated (see Table E-1.11.)
$X_{e,R}$	Unit soil loss from field (kg/m^2-yr)	Calculated (see Table E-1.28.)
A_F	Area of residential plot (m^2)	5,100
C_R	Constituent concentration in residential plot (mg/kg)	Calculated (see Table E-1.1.)
$X_{e,WS}$	Unit soil loss from the watershed (kg/m^2-yr)	Calculated (see Table E-4.6.)
A_{WS}	Total watershed area (m^2)	NA
SD_{WS}	Sediment delivery ratio for watershed (unitless)	Calculated (see Table E-4.7.)
C_{WS}	Watershed constituent concentration (mg/kg)	Calculated (see Table E-4.1.)

Description

This equation calculates the average concentration of delivered sediment for the watershed allowing for different unit soil loss factors and sediment delivery ratios for each of the modeled areas.

Table E-4.21. Total Waterbody Concentration

Fisher Scenario

$$C_{wtot} = \frac{L_T}{Vf_x \; x \; f_{water} + k_{wt} \; x \; WA_w \; x \; (d_w + d_b)}$$

Parameter	**Definition**	**Input Value**
C_{wtot}	Total water body concentration, including water column and bed sediment (mg/L) or (g/m^3)	
L_T	Total chemical load into water body; for overland transport, this includes deposition, runoff, and erosion; for groundwater pathways, this is the mass flux (M_{Flux}) to surface water (g/yr)	Calculated (for overland transport see Table E-4.10., for groundwater pathway see Table E-7.1. (M_{Flux})
Vf_x	Average volumetric flow rate through water body (m^3/yr)	Site specific
f_{water}	Fraction of total water body constituent concentration that occurs in the water column (unitless)	Calculated (see Table E-4.22.)
k_{wt}	Overall total waterbody dissipation rate constant (1/yr)	Calculated (see Table E-4.23.)
WA_w	Waterbody surface area (m^2)	Site specific
d_w	Depth of water column (m)	Site specific
d_b	Depth of upper benthic layer (m)	Site specific

Description

This equation calculates the total waterbody concentration, including both the water column and the bed sediment.

Table E-4.22. Fraction in Water Column and Benthic Sediment

Fisher Scenario

$$f_{water} = \frac{(1 + Kd_{sw}\ x\ TSS\ x\ 10^{-6})\ x\ d_w /\ d_z}{(1 + Kd_{sw}\ x\ TSS\ x\ 10^{-6})\ x\ d_w/d_z + (\theta_{bs} + Kd_{bs}\ x\ BS)\ x\ d_b\ /d_z}$$

$$f_{benth} = 1 - f_{water}$$

Parameter	Definition	Central Tendency	High End
f_{water}	Fraction of constituent concentration that occurs in the water column (unitless)		
Kd_{sw}	Suspended sediment/surface water partition coefficient (L/kg)	Chemical specific	
TSS	Total suspended solids (mg/L)	80	
10^{-6}	Conversion factor (kg/mg)		
d_w	Depth of the water column (m)	Site specific	
d_z	Total waterbody depth (m)	Calculated (d_w+d_b)	
d_b	Depth of the upper benthic layer (m)	Site specific	
θ_{bs}	Bed sediment porosity (L_{water}/L)	0.6	
Kd_{bs}	Bed sediment/sediment pore water partition coefficient (L/kg) or (g/cm^3)	Chemical-specific	
BS	Bed sediment concentration (g/cm^3)	1.0	
f_{benth}	Fraction of total waterbody constituent concentration that occurs in the benthic sediment (unitless)		

Description

These equations calculate the fraction of total waterbody concentration occurring in the water column and the bed sediments.

Table E-4.23. Overall Total Waterbody Dissipation Rate Constant

Fisher Scenario

$$k_{wt} = f_{water} \times k_v + k_b$$

Parameter	Definition	Central Tendency	High End
k_{wt}	Overall total waterbody dissipation rate constant (1/yr)		
f_{water}	Fraction of total waterbody constituent concentration that occurs in the water column (unitless)	Calculated (see Table E-4.22.)	
k_v	Water column volatilization rate constant (1/yr)	Calculated (see Table E-4.24.)	
k_b	Benthic burial rate constant (1/yr)	Calculated (see Table E-4.25.)	

Description

This equation calculates the overall dissipation rate of a constituent in surface water due to volatilization and benthic burial.

Table E-4.24. Water Column Volatilization Loss Rate Constant

Fisher Scenario

$$k_v = \frac{K_v}{d_z \; x \; (1 + Kd_{sw} \; x \; TSS \; x \; 10^{-6})}$$

Parameter	Definition	Central Tendency	High End
k_v	Water column volatilization rate constant (1/yr)		
K_v	Overall transfer rate (m/yr)	Calculated (see Table E-4.13.)	
d_z	Total waterbody depth (m)	Calculated (d_w+d_b)	
Kd_{sw}	Suspended sediment/surface water partition coefficient (L/kg)	Chemical specific	
TSS	Total suspended solids (mg/L)	80	
10^{-6}	Conversion factor (kg/mg)		

Description

This equation calculates the water column constituent loss due to volatilization.

Table E-4.25. Benthic Burial Rate Constant

Fisher Scenario

$$k_b = f_{benth} \; x \; \left(\frac{W_b}{d_b} \right)$$

Parameter	**Definition**	**Central Tendency**	**High End**
k_b	Benthic burial rate constant (1/yr)		
f_{benth}	Fraction of total waterbody constituent concentration that occurs in the benthic sediment	Calculated (see Table E-4.22)	
W_b	Burial rate (m/yr)	Calculated (see Table E-4.26)	
d_b	Depth of upper benthic sediment layer (m)	Site specific	

Description

This equation calculates the water column constituent loss due to burial in benthic sediment.

Table E-4.26. Benthic Burial Rate Constant

Fisher Scenario

$$W_b = W_{dep} \ \ x \ \ \left(\frac{TSS \ \ x \ \ 10^{-6}}{BS} \right)$$

Parameter	Definition	Central Tendency	High End
W_b	Benthic burial rate constant (m/yr)		
W_{dep}	Deposition rate to bottom sediment (m/yr)	Calculated (see Table E-4.27)	
TSS	Total suspended solids (mg/L)	80	
10^{-6}	Units conversion factor (kg/mg)		
BS	Bed sediments concentration (kg/L)	1	

Description

This equation is used to determine the loss of constituent from the benthic sediment layer.

Table E-4.27. Deposition Rate to Bottom Sediment

Fisher Scenario

$$W_{dep} = \left(\frac{X_{e,ws} \ x \ A_{ws} \ x \ SD_{ws} \ x \ 1000 - Vf_{x} \ x \ TSS}{WA_{w} \ x \ TSS} \right)$$

Parameter	Definition	Central Tendency	High End
W_{dep}	Deposition rate to bottom sediment (m/yr)		
$X_{e,ws}$	Unit soil loss from the watershed (kg/m^2-yr)	Calculated (see Table E-4.6)	
A_{ws}	Area of watershed (m^2)	NA	
SD_{ws}	Watershed sediment delivery ratio (unitless)	Calculated (see Table E-4.7)	
Vf_{x}	Average volumetric flow rate (m^3/yr)	Site specific	
TSS	Total suspended solids (g/m^3)	80	
1000	Units conversion factor (g/kg)		
WA_{w}	Waterbody surface area (m^2)	Site specific	

Description

This equation is used to determine the loss of a constituent from the waterbody as it deposits onto the benthic sediment.

Table E-4.28. Total Water Column Concentration

Fisher Scenario

$$C_{wt} = f_{water} \; x \; C_{wtot} \; x \; \frac{d_w + d_b}{d_w}$$

Parameter	Definition	Central Tendency	High End
C_{wt}	Total concentration in water column (mg/L)		
f_{water}	Fraction of total water body constituent concentration that occurs in the water column (unitless)	Calculated (see Table E-4.22.)	
C_{wtot}	Total water concentration in surface water system, including water column and bed sediment (mg/L)	Calculated (see Table E-4.21.)	
d_b	Depth of upper benthic layer (m)	Site specific	
d_w	Depth of the water column (m)	Site specific	

Description

This equation calculates the total water column concentration of a constituent; including both dissolved constituent and constituent sorbed to suspended solids.

Table E-4.29. Dissolved Water Concentration

Fisher Scenario

$$C_{dw} = \frac{C_{wt}}{1 + Kd_{sw} \; x \; TSS \; x \; 10^{-6}}$$

Parameter	Definition	Central Tendency	High End
C_{dw}	Dissolved phase water concentration (mg/L)		
C_{wt}	Total concentration in water column (mg/L)	Calculated (see Table E-4.28.)	
Kd_{sw}	Suspended sediment/surface water partition coefficient (L/kg)	Chemical specific	
10^{-6}	Units conversion factor (kg/mg)		
TSS	Total suspended solids (mg/L)	80	

Description

This equation calculates the concentration of constituent dissolved in the water column.

Table E-4.30. Concentration Sorbed to Bed Sediment

Fisher Scenario

$$C_{bs} = f_{benth} \ x \ C_{wtot} \ x \ \frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \ x \ BS} \ x \ \frac{d_w + d_b}{d_b}$$

Parameter	Definition	Central Tendency	High End
C_{bs}	Concentration sorbed to bed sediments (mg/kg)		
f_{benth}	Fraction of total waterbody constituent concentration that occurs in the bed sediment (unitless)	Calculated (see Table E-4.22.)	
C_{wtot}	Total water concentration in surface water system, including water column and bed sediment (mg/L)	Calculated (see Table E-4.21.)	
d_w	Total depth of water column (m)	Site specific	
d_b	Depth of the upper benthic layer (m)	Site specific	
θ_{bs}	Bed sediment porosity (unitless)	0.6	
Kd_{bs}	Bed sediment/sediment pore water partition coefficient (L/kg)	Chemical specific	
BS	Bed sediment concentration (kg/L)	1.0	

Description

This equation calculates the concentration of constituent sorbed to bed sediments.

Table E-4.31. Fish Concentration from Dissolved Water Concentration

Fisher Scenario

$$C_{fish} = C_{dw} \times BCF$$

Parameter	**Definition**	**Central Tendency**	**High End**
C_{fish}	Constituent concentration in fish tissue (mg/kg)		
C_{dw}	Dissolved water concentration (mg/L)	Calculated (see Table E-4.29.)	
BCF	Bioconcentration factor (L/kg)	Chemical specific	

Description

This equation calculates the constituent concentration if fish tissue as the product of the bioconcentration factor and the concentration dissolved in water.

Table E-4.32. Fish Concentration from Total Water Column Concentration

Fisher Scenario

$$C_{fish} = C_{wt} \ x \ BAF$$

Parameter	Definition	Central Tendency	High End
C_{fish}	Fish concentration (mg/kg)		
C_{wt}	Total water column concentration (mg/L)	Calculated (see Table E-4.28.)	
BAF	Bioaccumulation factor (L/kg)	Chemical specific	

Description

This equation calculates the constituent concentration if fish tissue as the product of the bioaccumulation factor and the total concentration in water.

Table E-5.1. Contaminant Intake from Soil

$$I_{soil} = S_c \cdot CR_{soil} \cdot f_{soil}$$

Parameter	Description	Values
I_{soil}	Daily intake of contaminant from soil (mg/d)	
S_c	Average soil concentration of pollutant over exposure duration (mg/kg)	calculated (see Table E-4.18.)
CR_{soil}	Consumption rate of soil (kg/d)	varies
f_{soil}	Fraction of consumed soil that is contaminated (unitless)	1

Description

This equation calculates the daily intake of contaminant from soil consumption. The soil concentration will vary with each scenario, and the soil consumption rate varies for children.

Table E-5.2. Contaminant Intake from Exposed Vegetable Intake

$$I_{ev} = (Pd + Pv + Pr) \cdot CR_{ev} \cdot f_{ev}$$

Parameter	Description	Values
I_{ev}	Daily intake of contaminant from exposed vegetables (mg/d)	
Pd	Concentration in exposed vegetables due to deposition (mg/kg DW)	calculated (see Table E-2.10 for Home Gardener, Table E-3.10 for the Farmer)
Pv	Concentration in exposed vegetables due to air-to-plant transfer (mg/kg DW)	calculated (see Table E-2.11 for Home Gardener, Table E-3.11 for the Farmer)
Pr	Concentration in exposed vegetables due to root uptake (mg/kg DW)	calculated (see Table E-2.12 for Home Gardener, Table E-3.12 for the Farmer)
CR_{ev}	Consumption rate of exposed vegetables (kg DW/d)	varies
f_{ev}	Fraction of exposed vegetables that are contaminated (unitless)	varies

Description

This equation calculates the daily intake of contaminant from ingestion of exposed vegetables on a dry weight (DW) basis. The consumption rate varies for children and adults. The contaminated fraction and the concentration in exposed vegetables will vary with each scenario.

Table E-5.3. Contaminant Intake from Exposed Fruit Intake

$$I_{ef} = (Pd + Pv + Pr) \cdot CR_{ef} \cdot f_{ef}$$

Parameter	Description	Values
I_{ef}	Daily intake of contaminant from exposed fruit (mg/d)	
Pd	Concentration in exposed fruit due to deposition (mg/kg DW)	calculated
Pv	Concentration in exposed fruit due to air-to-plant transfer (mg/kg DW)	calculated (see Table E-2.11 for Home Gardener, Table E-3.11 for the Farmer)
Pr	Concentration in exposed fruit due to root uptake (mg/kg DW)	calculated (see Table E-2.12 for Home Gardener, Table E-3.12 for the Farmer)
CR_{ef}	Consumption rate of exposed fruit (kg DW/d)	varies
f_{ef}	Fraction of exposed fruit contaminated (unitless)	varies

Description

This equation calculates the daily intake of contaminant from ingestion of exposed fruit on a dry weight (DW) basis. The consumption rate varies for children and adults. The contaminated fraction and the concentration in exposed fruit will vary with each scenario.

Table E-5.4. Contaminant Intake from Root Vegetable Intake

$$I_{rv} = Pr_{rv} \cdot CR_{rv} \cdot f_{rv}$$

Parameter	Description	Values
I_{rv}	Daily intake of contaminant from root vegetables (mg/d)	
Pr_{rv}	Concentration in root vegetables due to deposition, for organics (mg/kg - wet weight [WW]); metals (mg/kg - dry weight [DW])	calculated (see Table E-2.13 for Home Gardener, Table E-3.13 for the Farmer)
CR_{rv}	Consumption rate of root vegetables for organics (kg WW/d); metals (kg DW/d)	varies
f_{rv}	Fraction of root vegetables that are contaminated (unitless)	varies

Description

This equation calculates the daily intake of contaminant from ingestion of root vegetables. The consumption rate varies for children and adults. The contaminated fraction and the concentration in exposed vegetables will vary with each scenario.

Table E-5.5. Contaminant Intake from Beef and Dairy Intake

$$I_i = A_i \bullet CR_i \bullet f_i$$

Parameter	Description	Values
I_i	Daily intake of contaminant from animal tissue *i* (mg/d)	
A_i	Concentration in animal tissue *i* (mg/kg WW) - for Dioxins and (mg/kg DW) - for Cadmium	calculated (see Table E-3.14 for Beef, Table E-3.15 for dairy)
CR_i	Consumption rate of animal tissue *i* (kg WW/d) - for Dioxins and (Kg DW/d) - for Cadmium	varies
f_i	Fraction of animal tissue *i* that is contaminated (unitless)	varies

Description

This equation calculates the daily intake of contaminant from ingestion of animal tissue (where the "*i*" in the above equation refers to beef and dairy). The consumption rate varies for children and adults and for the type of animal tissue.

Table E-5.6. Contaminant Intake from Fish Intake

$$I_{fish} = C_{fish} \bullet CR_{fish} \bullet f_{fish}$$

Parameter	Description	Values
I_{fish}	Daily intake of contaminant from fish (mg/d)	
C_{fish}	Concentration in fish (mg/kg)	calculated (see Tables E-4.31 and E-4.32)
CR_{fish}	Consumption rate of fish (kg/d)	varies
f_{fish}	Fraction of fish that are contaminated (unitless)	varies

Description

This equation calculates the daily intake of contaminant from ingestion of fish.

Table E-5.7. Total Daily Intake for Non-groundwater Indirect Pathways

Adult Resident and Child of Resident

$$I = I_{soil}$$

Home Gardener

$$I = I_{soil} + I_{ev} + I_{ef} + I_{rv}$$

Farmer and Child of Farmer

$$I = I_{soil} + I_{ev} + I_{beef} + I_{dairy} + I_{ef} + I_{rv}$$

Fisher

$$I = I_{fish}$$

Parameter	Description	Values
I	Total daily intake of contaminant (mg/d)	
I_{soil}	Daily intake of contaminant from soil (mg/d)	calculated (see Table E-5.1)
I_{ev}	Daily intake of contaminant from exposed vegetables	calculated (see Table E-5.2)
I_{ef}	Daily intake of contaminant from exposed fruit (mg/d)	calculated (see Table E-5.3)
I_{rv}	Daily intake of contaminant from root vegetables	calculated (see Table E-5.4)
I_{beef}, I_{dairy}	Daily intake of contaminant from animal tissue (mg/d)	calculated (see Table E-5.5)
I_{fish}	Daily intake of contaminant from fish (mg/d)	calculated (see Table E-5.6)

Description

These equations calculate the daily intake of contaminant on a pathway by pathway basis.

Table E-5.8. Individual Cancer Risk: Carcinogens

$$CancerRisk = \frac{I \cdot ED \cdot EF \cdot CSF}{BW \cdot AT \cdot 365}$$

Parameter	Description	Values
Cancer Risk	Individual lifetime cancer risk (unitless)	
I	Total daily intake of contaminant (mg/d)	calculated (see Tables E-5.1 - E-5.6)
ED	Exposure duration (yr)	varies
EF	Exposure frequency (d/yr)	350
BW	Body weight (kg)	adult: 70 child: varies
AT	Averaging time (yr)	70
365	Units conversion factor (d/yr)	
CSF	Oral cancer slope factor $(mg/kg/d)^{-1}$	chemical-specific

Description

This equation calculates the individual cancer risk from indirect exposure to carcinogenic chemicals. The body weight varies for the child. The exposure duration varies for different scenarios.

Table E-5.9. Hazard Quotient: Noncarcinogens

$$HQ = \frac{I}{BW \cdot RfD}$$

Parameter	Description	Values
HQ	Hazard quotient (unitless)	
I	Total daily intake of contaminant (mg/d)	calculated (see Tables E-5.1 - E-5.6)
BW	Body weight (kg)	adult: 70 child: varies
RfD	Reference Dose (mg/kg/d)	chemical-specific

Description

This equation calculates the hazard quotient for indirect exposure to non-carcinogenic chemicals. The body weight varies for the child.

Table E-6.1 Concentration in Air

$$C_a = (C_{vapor} \bullet J_{air,t}) + (PM_{10} \bullet C_0 \bullet C_{particulate} \bullet \frac{1}{1000} \bullet \frac{1}{1000}$$

Parameter	Description	Values
C_a	Concentration in air (μg/m^3)	
C_{vapor}	Annual average vapor concentration per unit flux ((μg/m^3)/(g/m^2-s))	Modeled ISC3
$J_{air,t}$	Total contaminant flux to the atmosphere (g/m^2-s)	Modeled (chemical-specific)
PM_{10}	Particulate matter (<10 micrometers) flux to the atmosphere (g/m^2-s)	Modeled
C_0	Source constituent concentration (mg/kg)	chemical-specific
$C_{particulate}$	Annual average particulate concentration per unit flux ((μg/m^3)/(g/m^2-s))	Modeled ISC3

Description

This equation calculates the air concentration of constituents at the exposure point

Table E-6.2. Inhalation Cancer Risk for Individual Chemicals from Unit Risk Factor: Carcinogens

$$Cancer\,Risk = C_a \bullet URF$$

Parameter	Description	Values
Cancer Risk	Individual lifetime cancer risk (unitless)	
C_a	Concentration in air (μg/m^3)	calculated (see Table E-6.1)
URF	Inhalation unit risk factor (μg/m^3)$^{-1}$	chemical-specific

Description

This equation calculates the inhalation cancer risk for individual constituents using the unit risk factor.

Table E-6.3. Inhalation Cancer Risk for Individual Chemicals from Carcinogenic Slope Factor: Carcinogens

$$CSF_{inh} = \frac{URF \bullet 1000 \bullet 70}{20}$$

$$CancerRisk = ADI \bullet CSF_{inh}$$

$$ADI = \frac{C_a \bullet IR \bullet ET \bullet EF \bullet ED \bullet 0.001\ mg/\mu g}{BW \bullet AT \bullet 365\ day/yr}$$

Parameter	Description	Values
Cancer Risk	Individual lifetime cancer risk (unitless)	
URF	Inhalation unit risk factor $(\mu g/m^3)^{-1}$	chemical specific
ADI	Average daily intake via inhalation (mg/kg/day)	calculated
C_a	Concentration of contaminant in the air $(\mu g/m^3)$	calculated (see Table E-6.1)
IR	Inhalation rate (m^3/hr)	varies
ET	Exposure time (hr/day)	24
EF	Exposure frequency (day/yr)	350
ED	Exposure Duration (yr)	varies
BW	Body weight (kg)	Adult = 70 Child = varies
AT	Averaging time (yr)	70
CSF_{inh}	Inhalation carcinogenic slope factor $(mg/kg/day)^{-1}$	chemical-specific
1000	Unit conversion (µg/mg)	
70	Default adult body weight (kg)	
20	Default adult daily inhalation rate (m^3/d)	

Description
These equations calculate the inhalation cancer slope factor from the unit risk factor and the inhalation cancer risk for individual constituents using the cancer slope factor.

Table E-6.4. Inhalation Hazard Quotient for Individual Chemicals: Noncarcinogens

$$HQ = \frac{C_a \bullet 0.001\ mg/\mu g}{RfC}$$

Parameter	Description	Values
HQ	Hazard quotient (unitless)	
C_a	Concentration in air ($\mu g/m^3$)	calculated (see Table E-6.1.)
RfC	Reference concentration (mg/m^3)	chemical-specific

Description

This equation calculates the inhalation hazard quotient for individual constituents.

Table E-7.1. Calculation of Groundwater to Surface Water Mass Flux, Landfills and Land Treatment Units, all Constituents of Concern

Chlorinated Aliphatics, Landfill & Land Treatment Unit Scenarios

$$M_{Flux} = i \ x \ K_H \ x \ c_{net}$$

Parameter	Definition	Central Tendency	High End
M_{Flux}	Total contaminant mass flux (mg/yr)		
i	Hydraulic gradient (unitless)	0.005	
K_H	Hydraulic conductivity (m/yr)	1580	
c_{net}	Net contaminant mass in plume cross-section perpendicular to groundwater flow direction (mg/m)	calculated (see Table E-7.2)	

Description

This equation is used for the groundwater to surface water pathway to calculate the contaminant mass flux at a given downgradient location. This location represents the intersection of the contaminant plume with a surface waterbody. It is assumed that the surface water body fully penetrates the aquifer and the plume fully intersects the waterbody.

Table E-7.2. Calculation of the Net Contaminant Mass in the Plume, Landfills and Land Treatment Units, all Constituents of Concern

Chlorinated Aliphatics, Landfill & Land Treatment Unit Scenarios

$$c_{net} = F \times [\int C(y)\ dy]$$

Parameter	Definition	Central Tendency	High End
c_{net}	Net contaminant mass in plume cross-section perpendicular to groundwater flow direction (mg/m)		
F	Conversion factor (L/m^3)	1000	
C(y)	Contaminant concentration as a function of the transverse distance from plume centerline (mg-m/L)	calculated (see Table E-7.3)	
$\int C(y)\ dy$	Integral of the contaminant concentration as a function of transverse distance from the plume centerline (y=0) to the plume boundary (y=plume), in (mg-m^2/L)	calculated (see Table E-7.3)	

Description

This equation is used to calculate the net contaminant mass by integrating the transverse contaminant concentration from the plume centerline to the plume boundary.

Table E-7.3. Calculation of the Contaminant Concentration, Landfills and Land Treatment Units, all Constituents of Concern

Chlorinated Aliphatics, Landfill & Land Treatment Unit Scenarios

$$C(y) = [\ \frac{(c_{avg}\ x\ ZB)}{2}\ x \int (f(y)\ dy)\ ]$$

Parameter	Definition	Central Tendency	High End
C(y)	Contaminant concentration as a function of the transverse distance from plume centerline (mg m/L)		
c_{avg}	Average receptor well concentration (mg/L)	chemical-specific	
ZB	Saturated zone thickness (m)	9.14	
f(y)	Function of the transverse distance from plume centerline	calculated (see Table E-7.5)	
$\int f(y)\ dy$	integral of the transverse distance from the plume centerline to the plume boundary (m)	calculated (see Table E-7.4)	

Description

This equation is used to approximate the contaminant concentration as a function of transverse distance (Domenico and Schwartz, 1990).

Table E-7.4. Calculation of the Integral of the Transverse Distance from Plume Centerline, Landfills and Land Treatment Units, all Constituents of Concern

Chlorinated Aliphatics, Landfill & Land Treatment Unit Scenarios

$$\int f(y)\ dy = \frac{2\ h}{45}\ x\ [\ 7\ f(y_0) + 32\ f(y_1) + 12\ f(y_2) + 32\ f(y_3) + 7\ f(y_4)\ ]$$

Parameter	Definition	Central Tendency	High End
$\int f(y)\ dy$	Integral of the transverse distance from the plume centerline to the plume boundary (m)		
h	Interval between y_0 and y_1; y_1 and y_2; etc.	y-location-specific	
$f(y_i)$	Function of the transverse distance from plume centerline for specific y-locations y_0, y_1, y_2, y_3, y_4	y-location-specific	

Description

This equation is used to estimate the value of the integral using Simpson's 3/8 rule. This numerical method is applied because a closed form solution is not available (Burden and Faires, 1985).

Table E-7.5. Calculation of the Transverse Distance from Plume Centerline, Landfills and Land Treatment Units, all Constituents of Concern

Chlorinated Aliphatics, Landfill & Land Treatment Unit Scenarios

$$f(y) = erf\left[\frac{y + \frac{ys}{2}}{2\sqrt{\alpha_T\, x}}\right] - erf\left[\frac{y - \frac{ys}{2}}{2\sqrt{\alpha_T\, x}}\right]$$

Parameter	Definition	Central Tendency	High End
f(y)	Function of the transverse distance from plume centerline		
y	Transverse distance from plume centerline to point of interest within plume (m)		
ys	Source width (m)	plume size-specific	
α_T	Transverse dispersivity (m)	1.04	0.66=HE(x) 1.04=HE(y)
x	Downgradient distance from source (m)	430	102

Description

This equation is used to calculate the transverse distance from the plume center line to the point of interest within the plume (Domenico and Schwartz, 1990).

Table E-7.6. Calculation of Waste Concentration after Volatilization for Organic Constituents of Concern in Landfills

Chlorinated Aliphatics, Landfill Scenarios

$$C_{W(AV)} = \frac{M_{C(AV)}}{M_{T(AV)}}$$

$$M_{C(AV)} = (C_{W(BV)} \quad BD \quad V_W) - M_V$$

$$M_{T(AV)} = (BD \quad V_W) - M_V$$

Parameter	Definition	Central Tendency	High End
$C_{W(AV)}$	Waste concentration after volatilization (mg/Kg)		
$M_{C(AV)}$	Contaminant mass after volatilization (mg)		
$M_{T(AV)}$	Total mass of waste after volatilization (Kg)		
$C_{W(BV)}$	Average waste concentration before volatilization (mg/Kg), wet-weight basis	chemical-specific	
BD	Bulk density of waste (g/cm^3)	1.07	
V_W	Waste volume (m^3)	15201.87	50579.44
M_V	Contaminant mass volatilized during first 30 years of landfill operation (mg)	chemical-specific	

Description

These equations are used to calculate the waste concentration at the time the landfill is closed, that is, after 30 years. Volatilization is assumed to occur only during the active life of the landfill, prior to installation of clay cap. This waste concentration which is adjusted for volatilization losses is then used as input for the groundwater fate and transport modeling.

Table E-7.7. Calculation of Hydrolysis Rates from Hydrolysis Rate Constants for Organic Constituents of Concern in Landfills and Land Treatment Units

Chlorinated Aliphatics, Landfill and Land Treatment Unit Scenarios

$$\lambda = \frac{\lambda_1 \Phi + \lambda_2 BD K_d}{\Phi + BD K_d}$$

$$\lambda_1 = K_a^T 10^{-pH} + K_n^T + K_b^T 10^{-(14-pH)}$$

$$\lambda_2 = 10 K_a^T 10^{-pH} + K_n^T$$

Parameter	Definition	Central Tendency	High End
λ	Overall first-order chemical decay coefficient (1/yr)		
λ_1	Dissolved phase decay coefficient (1/yr)		
λ_2	Sorbed phase decay coefficient (1/yr)		
Φ	Effective porosity in saturated zone or saturated water content in the unsaturated zone	soil- and aquifer-specific (see table below)	
BD	Bulk density of soil (g/cm^3)	1.51	1.46
K_d	Soil-water partition coefficient (cm^3/g)	chemical-specific	
K_a^T	Acid-catalyzed hydrolysis rate constant at 25 °C (1/M·yr)	chemical-specific (see table below)	
K_n^T	Neutral hydrolysis rate constant 25 °C (1/yr)	chemical-specific (see table below)	
K_b^T	Base-catalyzed hydrolysis rate constant at 25 °C (1/M·yr)	chemical-specific (see table below)	
pH	Aquifer pH (standard units)	7.1	

Description

The equations above are used to calculate the overall chemical decay coefficient from the chemical-specific hydrolysis rate constants. In the EPACMTP model, the overall first-order chemical decay coefficient of an organic species is a combination of dissolved phase and sorbed phase decay (U.S. EPA,1996). The sorbed and dissolved phase decay coefficients are functions of the temperature-dependent chemical-specific hydrolysis rate constants K_a^T, K_n^T, K_b^T (U.S. EPA, 1996). The input values for neutral, acid, and base rate constants for each modeled chemical of concern are listed below.

Chemical Hydrolysis Rates (Kollig, 1993)			
Constituent	K_n^{25} (1/M·yr)	K_a^{25} (1/M·yr)	K_b^{25} (1/M·yr)
1,2-Dichloroethane	9.31E-3	0.0	54.7
Cis-1,3-Dichloropropene	40.0	0.0	0.0
Bis(2-Chloroethyl)ether	0.23	0.0	0.0
2-(2-Chloroethoxyl)ethanol	0.28	0.0	0.0
p-Dioxane	0.0	0.0	0.0
Chloroform	1.0E-4	0.0	2.74E+3
Methylene Chloride	1.0E-3	0.0	6.0E-1

Parameter	Landfill		Land Treatment Unit	
	CT	HE	CT	HE
Effective Porosity, saturated zone	0.24		0.24	
Saturated Water Content, unsaturated zone	0.43	0.45	0.45	

Table E-7.8. Calculation of Linear Isotherm for Arsenic, Landfills and Land Treatment Units

Chlorinated Aliphatics, Landfill and Land Treatment Unit Scenarios

$$K_d = 10^{(0.0322\,pH \;+\; 1.24)}$$

Parameter	Definition	Central Tendency	High End
K_d	Soil-water partition coefficient (cm^3/g)		
pH	Aquifer pH	7.1	

Description

Arsenic was modeled using an empirical pH-dependent adsorption isotherm (Loux et al., 1990).

Table E-7.9. Calculation of Linear Isotherm for Chromium (+6), Landfills and Land Treatment Units

Chlorinated Aliphatics, Landfill and Land Treatment Unit Scenarios			
$K_d = 10^{(-0.117\,pH + 2.07)}$			
Parameter	Definition	Central Tendency	High End
Kd	Soil-water partition coefficient (cm^3/g)		
pH	Aquifer pH	7.1	
Description			
Chromium (+6) was modeled using an empirical pH-dependent adsorption isotherm (Loux et al., 1990).			

Table E-7.10. Calculation of Linear Isotherm for Molybdenum, Landfills

Chlorinated Aliphatics, Landfill and Land Treatment Unit Scenarios			
$K_d = 10^{(-0.117\, pH \;+\; 2.07)}$			
Parameter	Definition	Central Tendency	High End
K_d	Soil-water partition coefficient (cm^3/g)		
pH	Aquifer pH	7.1	
Description			
Molybdenum was modeled using the Chromium (+6) pH-dependent adsorption isotherm (Loux et al., 1990).			

Table E-7.11. Calculation of Soil-Water Partition Coefficients for Organic Constituents of Concern, Landfills and Land Treatment Units

Chlorinated Aliphatics, Landfill and Land Treatment Unit Scenarios

$$K_d = k_{oc} \times f_{oc}$$

Parameter	Definition	Central Tendency	High End
K_d	Soil-water partition coefficient (cm^3/g)		
k_{oc}	Normalized distribution coefficient for organic carbon (cm^3/g)	chemical-specific (see table below)	
f_{oc}	Fractional organic carbon content	soil-specific	

Description

This equation is used to calculate the soil-water partition coefficient for organic constituents.

Chemical-specific Organic Carbon Content (Kollig, 1993)

Constituent	k_{oc} (cm^3/g)
1,2-Dichloroethane	13.49
Cis-1,3-Dichloropropene	63.1
Bis(2-Chloroethyl)ether	6.31
2-(2-Chloroethoxyl)ethanol	0.65
p-Dioxane	0.15
Chloroform	38.02
Methylene Chloride	8.51

Table E-7.12. Overall Mass Transfer Coefficient from Tap-Water to Air

All Exposure Scenarios

$$K_{ol} = \beta \ x \left(\frac{2.5}{D_1^{2/3}} + \frac{1}{D_a^{2/3} H'} \right)^{-1}$$

Parameter	Definition	Central Tendency	High End
K_{ol}	Overall mass transfer coefficient (cm/sec)		
β	Proportionality constant $(\mathrm{cm/sec})^{-1/3}$	216	
D_1	Diffusion coefficient in water ($\mathrm{cm^2/sec}$)	Chemical-specific	
D_a	Diffusion coefficient in air ($\mathrm{cm^2/sec}$)	Chemical-specific	
H'	Dimensionless Henry's law constant = 41 x H_{LC}	Chemical-specific	

Description

This equation is used to calculate constituents' overall mass transfer coefficient from tap-water to air from showering.

Table E-7.13. Dimensionless Overall Mass Transfer Coefficient

All Exposure Scenarios
$N = K_{ol} \; x \left(\frac{6}{d_p} \right) \; x \left(\frac{h}{v_t} \right)$

Parameter	Definition	Value
N	Dimensionless overall mass transfer coefficient (unitless)	
K_{ol}	Overall mass transfer coefficient (cm/sec)	Calculated
d_p	Droplet diameter (cm)	0.098
h	Nozzle height (cm)	180
v_t	Terminal velocity (cm/sec)	400

Description
This equation is used to calculate the dimensionless overall mass transfer coefficient from tap-water to air from showering.

Table E-7.14. Fraction of Constituent Emitted from Tap-water

All Exposure Scenarios		
$f_{em} = (1 - f_{sat})\ x\ (1 - e^{-N})$		
Parameter	**Definition**	**Value**
f_{em}	Fraction of constituent emitted from the tap-water (unitless)	
f_{sat}	Fraction of gas phase saturation (unitless)	Calculated
N	Dimensionless overall mass transfer coefficient (unitless)	Calculated
Description		
This equation is used to calculate the fraction of constituent that is emitted from tap water.		

Table E-7.15. Fraction of Gas Phase Saturation in the Shower

All Exposure Scenarios		
$$f_{sat,t} = \frac{y_{s,t}}{H' \times C_{in}}$$		
Parameter	**Definition**	**Value**
$f_{sat,t}$	Fraction of gas phase saturation (unitless)	
$y_{s,t}$	Gas phase constituent concentration in the shower at end of time step (mg/L)	Calculated
H'	Dimensionless Henry's law constant = 41 x H_{LC}	Chemical-specific
C_{in}	Constituent concentration in tap-water (mg/L)	Chemical-specific
Description		
This equation is used to calculate the fraction of gas phase saturation.		

Table E-7.16. Gas Phase Constituent Concentration in Shower

All Exposure Scenarios

$$y_{s,t+1} = y_{s,t} + (Q_{gs}\ x\ (y_{b,t} - y_{s,t})\ x\ (t_{t+1} - t_t) + E_{s,t})/V_s$$

Parameter	Definition	Value
$y_{s,t+1}$	Gas phase constituent concentration in the shower at end of time step (mg/L)	
$y_{s,t}$	Gas phase constituent concentration in the shower at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
Q_{gs}	Volumetric gas exchange rate between shower and bathroom (L/min)	100
$y_{b,t}$	Gas phase constituent concentration in the bathroom at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
$(t_{t+1} - t_t)$	Calculational time step (min)	0.2
$E_{s,t}$	Mass of constituent emitted from shower between time t and time t+1 (mg)	Calculated
V_s	Volume of shower stall (L)	2,300

Description

This equation is used to calculate the gas phase constituent concentration in the shower for each time step.

Table E-7.17. Gas Phase Constituent Concentration in Bathroom

All Exposure Scenarios

$$y_{b,t+1} = y_{b,t} + \left[(Q_{gs}\ x\ (y_{s,t} - y_{b,t})) - (Q_{gb}\ x\ (y_{b,t} - y_{h,t})) + (I_b\ x\ C_{in}\ x\ f_{em,b})\right]\ x \left(\frac{t_{t+1} - t_t}{V_b}\right)$$

Parameter	Definition	Value
$y_{b,t+1}$	Gas phase constituent concentration in the bathroom at end of time step (mg/L)	
$y_{b,t}$	Gas phase constituent concentration in the bathroom at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
Q_{gs}	Volumetric gas exchange rate between shower and bathroom (L/min)	100
$y_{s,t}$	Gas phase constituent concentration in the shower at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
Q_{gb}	Volumetric gas exchange rate between bathroom and house (L/min)	300
$y_{h,t}$	Gas phase constituent concentration in the bathroom at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
$(t_{t+1} - t_t)$	Calculational time step (min)	0.2
I_b	Bathroom water use (L/min)	2.08[(a)]
C_{in}	Constituent concentration in tap-water (mg/L)	Chemical-specific
$f_{em,b}$	Fraction of constituent emitted from bathroom water use (unitless)	0.5
V_b	Volume of bathroom (L)	13,600

Description

This equation is used to calculate the gas phase constituent concentration in the bathroom for each time step.

(a) Calculated based on total bathroom water use of 125 L/day and exposure duration in bathroom of 1 hr/day.

Table E-7.18. Gas Phase Constituent Concentration in House

All Exposure Scenarios

$$y_{h,t+1} = y_{h,t} + \left[(Q_{gb}\ x\ (y_{b,t} - y_{h,t}))\ -\ (Q_{gh}\ x\ (y_{h,t}\ -\ y_{a,t}))\ +\ (I_h\ x\ C_{in}\ x\ f_{em,h})\right]\ x\ \left(\frac{t_{t+1} - t_t}{V_h}\right)$$

Parameter	Definition	Value
$y_{h,t+1}$	Gas phase constituent concentration in the house at end of time step (mg/L)	
$y_{h,t}$	Gas phase constituent concentration in the house at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
Q_{gb}	Volumetric gas exchange rate between the bathroom and house (L/min)	300
$y_{b,t}$	Gas phase constituent concentration in the bathroom at beginning of time step (mg/L)	Calculated (0.00 for 1st time step)
Q_{gh}	Volumetric gas exchange rate between house and atmosphere (L/min)	2,325
$y_{a,t}$	Gas phase constituent concentration in the atmosphere (mg/L)	assumed 0.00
$(t_{t+1} - t_t)$	Calculational time step (min)	0.2
I_h	Water use in house - other than bathroom (L/min)	0.21$^{(a)}$
C_{in}	Constituent concentration in tap-water (mg/L)	Chemical-specific
$f_{em,h}$	Fraction of constituent emitted from household water use - other than bathroom (unitless)	0.66
V_h	Volume of house (L)	310,000

Description

This equation is used to calculate the gas phase constituent concentration in the house for each time step.

(a) Calculated based on total bathroom water use of 201 L/day and 16 hours of household exposure.

Table E-7.19. Average Air Concentration in Shower

All Exposure Scenarios

$$C_{avg,s} = \frac{\sum_{t=1}^{N} y_{s,t}}{n}$$

Parameter	Definition	Value
$C_{avg,s}$	Average air concentration in shower (mg/L)	
t	Calculational time step index	0.2
N	Total number of time steps over the duration of the shower	57
n	Total time in shower (min)	11.4
$y_{s,t}$	Gas phase constituent concentration in the shower at time t (mg/L)	Calculated

Description

This equation is used to calculate the average air concentration in the shower for the showering period.

Table E-7.20. Average Air Concentration in Bathroom

All Exposure Scenarios

$$C_{avg,b} = \frac{\sum_{t=1}^{N} y_{b,t}}{n}$$

Parameter	Definition	Value
$C_{avg,b}$	Average air concentration in bathroom (mg/L)	
t	Calcutational time step index	0.2
N	Total number of time steps for the time in the bathroom excluding time in shower	243
n	Total time in bathroom excluding time in shower (min)	48.6
$Y_{b,t}$	Air concentration in bathroom at end of time t (mg/L)	Calculated

Description

This equation is used to calculate the average air concentration for the period in the bathroom excluding the showering period.

Table E-7.21. Dose Absorbed per Unit Area per Event

All Exposure Scenarios		
$DA_{event} = C_{water}\ x\ K_p^w \left[\frac{t_{event}}{1+B} + 2\tau \left(\frac{1+3B}{1+B} \right) \right] x\ 0.001$		
Parameter	**Definition**	**Value**
DA_{event}	Dose absorbed per unit area per event (mg/cm^2-event)	
C_{water}	Water concentration (mg/L)	Calculated
K_p^w	Skin permeability constant in water (cm/h)	chemical-specific
t_{event}	Duration of event (h)	0.167
τ	Lag time (h)	chemical-specific
B	Bunge constant (unitless)	chemical-specific
0.001	Unit conversion factor (L/cm^3)	
Description		
This equation is used to calculate the contaminant dose from showering.		

Table E-7.22. Cancer Risk for Dermal Exposure to Tap Water

Adult Exposure Scenarios

$$Cancer\,Risk = \frac{DA_{event}\,x\,EF\,x\,EF_{event}\,x\,ED\,x\,SA_{skin}\,x\,Adjusted\,CSF}{AT\,x\,365\,days/yr\,x\,BW}$$

Parameter	Definition	Value
Cancer Risk	Individual lifetime cancer risk (unitless)	
DA_{event}	Dose absorbed per unit area per event (mg/cm^2-event)	calculated (see Table E-7.21)
EF	Exposure frequency (days/yr)	350
EF_{event}	Event exposure frequency (showers per day) (event/day)	1
ED	Exposure duration (yr)	varies
SA_{skin}	Surface area of skin (cm^2)	20,000
Adjusted CSF[a]	Cancer slope factor (mg/kg/day)$^{-1}$	chemical-specific
AT	Averaging time (yrs)	70
BW	Body weight (kg)	Adult = 70

Description

This equation is used to calculate the cancer risk for dermal exposure to tap water.

[a] The Adjusted CSF is calculated by dividing the oral CSF by the oral absorption efficiency for the appropriate chemical type. The following oral absorption efficiencies were used in this analysis:

80% for Volatile organic chemicals
50% for Semi-volatile organic chemicals
20% for Metals

Table E-7.23. Hazard Quotient for Dermal Exposure to Tap Water

Adult Exposure Scenarios

$$HQ = \frac{DA_{event}\ x\ EF_{event}\ x\ SA_{skin}}{Adjusted\ RfD\ x\ BW}$$

Parameter	Definition	Value
HQ	Hazard quotient for dermal exposure to tap water (unitless)	
DA_{event}	Dose absorbed per unit area per event (mg/cm^2-event)	calculated (see Table E-7.21)
EF_{event}	Event exposure frequency (showers per day) (event/day)	1
SA_{skin}	Surface area of skin (cm^2)	20,000
Adjusted RfD[a]	Oral reference dose (mg/kg/day)	chemical-specific
BW	Body weight (kg)	Adult = 70

Description

This equation is used to calculate the hazard quotient for dermal exposure to tap water.

[a] The Adjusted RfD is calculated by dividing the RfD by the oral absorption efficiency for the appropriate chemical type. The following oral absorption efficiencies were used in this analysis:

80% for Volatile organic chemicals
50% for Semi-volatile organic chemicals
20% for Metals

Table E-7.24. Contaminant Intake from Drinking Water Intake

$$I_{dw} = C_{dw} \; x \; CR_{dw} \; x \; f_{dw}$$

Parameter	Description	Values
I_{dw}	Daily intake of contaminant from drinking water (mg/d)	
C_{dw}	Concentration in well water (mg/L)	calculated
CR_{dw}	Consumption rate of drinking water (L/d)	varies
f_{dw}	Fraction of drinking water contaminated (unitless)	varies

Description
This equation calculates the daily intake of contaminant from ingestion of drinking water.

Table E-7.25. Contaminant Intake from Fish Intake (Discharge of Groundwater to Surface Water)

$$I_{fish} = C_{fish} \, x \, CR_{fish} \, x \, f_{fish}$$

Parameter	Description	Values
I_{fish}	Daily intake of contaminant from fish (mg/d)	
C_{fish}	Concentration in fish (mg/kg)	calculated (see Tables E-4.31 and E-4.32.)
CR_{fish}	Consumption rate of fish (kg/d)	varies
f_{fish}	Fraction of fish contaminated (unitless)	varies

Description
This equation calculates the daily intake of contaminant from ingestion of fish.

Table E-7.26. Individual Cancer Risk from Ingestion: Carcinogens

$$CancerRisk = \frac{I \cdot ED \cdot EF \cdot CSF}{BW \cdot AT \cdot 365}$$

Parameter	Description	Values
Cancer Risk	Individual lifetime cancer risk (unitless)	
I	Total daily intake of contaminant (mg/d)	calculated (see Tables E-5.1 - E-5.6)
ED	Exposure duration (yr)	varies
EF	Exposure frequency (day/yr)	350
BW	Body weight (kg)	adult: 70 child: varies
AT	Averaging time (yr)	70
365	Units conversion factor (d/yr)	
CSF	Oral cancer slope factor (per mg/kg/d)	chemical-specific

Description

This equation calculates the individual cancer risk from tap water ingestion of carcinogenic chemicals. The body weight varies for the child. The exposure duration varies for different scenarios.

Table E-7.27. Hazard Quotient: Noncarcinogens

$$HQ = \frac{I}{BW \cdot RfD}$$

Parameter	Description	Values
HQ	Hazard quotient (unitless)	
I	Total daily intake of contaminant (mg/d)	calculated (see Tables E-5.1 - E-5.6)
BW	Body weight (kg)	adult: 70 child: varies
RfD	Reference Dose (mg/kg/d)	chemical-specific

Description

This equation calculates the hazard quotient for indirect exposure to noncarcinogenic chemicals. The body weight varies for the child.

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