

APPENDIX F

**SUMMARY OF DATA SOURCES FOR PARAMETERS USED IN THE MULTIPLE PATHWAY
HEALTH RISK ASSESSMENT**

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Acronyms and Abbreviations

Acronym/ Abbreviation	Definition
θ	temperature correction factor
θ_{bs}	bed sediment porosity
θ_{sw}	soil volumetric water content
λ_z	dimensionless viscous sublayer thickness
μ_a	viscosity of air corresponding to air temperature
μ_w	viscosity of water corresponding to water temperature
ρ_a	density of air
ρ_{soil}	solids particulate density
ρ_{forage}	density of forage
ρ_w	density of water
τ_{event}	lag time per event
A	body surface area exposed during swimming
a	empirical intercept coefficient
ABS_d	dermal absorption fraction
ABS_{GI}	fraction of contaminant absorbed in the gastrointestinal tract
AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model
AF	soil adherence factor
A_I	impervious watershed area receiving chemical deposition
A_L	total watershed area receiving chemical deposition
AT_{carc}	averaging time for carcinogenic effects
$AT_{noncarc, direct}$	averaging time for noncarcinogenic direct pathways
$AT_{noncarc, indirect}$	averaging time for noncarcinogenic indirect pathways
A_w	water body surface area
atm	atmosphere
atm-m ³ /mol	atmosphere-cubic meter(s) per mole
ATSDR	Agency for Toxic Substances and Disease Registry
b	empirical slope coefficient and correlation coefficient b
B	dimensionless ratio of the permeability coefficient through the stratum corneum relative to the permeability coefficient across the viable epidermis
Ba_{beef}	biotransfer factor for beef
Ba_{chick}	biotransfer factor for chicken
Ba_{egg}	biotransfer factor for eggs

Acronym/ Abbreviation	Definition
Ba_{fat}	biotransfer factor for fat
BAF_{fish}	bioaccumulation factor
Ba_{milk}	biotransfer factor for milk
Ba_{pork}	biotransfer factor for pork
BCF_{fish}	bioconcentration factor
BD	soil bulk density
BEHP	bis(2-ethylhexyl)phthalate
Br_{ag}	plant-to-soil bioconcentration factor for above-ground produce
Bs	soil bioavailability factor
$BSAF_{fish}$	biota-to-sediment accumulation factor
Bv_{ag}	air-to-plant biotransfer factor
B_{vol}	volumetric air-to-plant biotransfer factor
BW	body weight
c	Junge constant and correlation coefficient c
C	USLE cover management factor
C_{BS}	bed sediment concentration
C_d	drag coefficient
cm/yr	centimeter(s) per year
COPC	chemical of potential concern
CR_{beef}	consumption rate of beef
CR_{bg}	consumption rate of below-ground vegetables
CR_{chick}	consumption rate of chicken
CR_{egg}	consumption rate of eggs
$CR_{exposed\ fruit}$	consumption rate of exposed fruit
$CR_{exposed\ veg}$	consumption rate of exposed vegetables
CR_{fish}	consumption rate of fish
CR_{milk}	consumption rate of dairy milk
CR_{pork}	consumption rate of pork
$CR_{protected\ fruit}$	consumption rate of protected fruit
$CR_{protected\ veg}$	consumption rate of protected vegetables
CR_{soil}	consumption rate of soil
CR_{sw}	incidental consumption rate of surface water
Cyp	particle phase air concentration
Cyv	vapor phase air concentration
Cyvw	watershed vapor phase air concentration

Acronym/ Abbreviation	Definition
D_a	diffusivity of chemical in air
d_{bs}	depth of upper benthic layer
DOC	dissolved organic carbon
D_{sc}	effective diffusion coefficient for chemical transfer through the stamum corneum
D_w	diffusivity of chemical in water
d_{wc}	depth of water column
$Dydp$	yearly dry deposition from particle phase
$Dydv$	yearly dry deposition from vapor phase
$Dywdp$	yearly watershed dry deposition from particle phase
$Dywdv$	yearly watershed dry deposition from vapor phase
$Dywp$	yearly wet deposition from particle phase
$Dyww$	yearly wet deposition from vapor phase
$Dywwp$	yearly watershed wet deposition from particle phase
$Dywwv$	yearly watershed wet deposition from vapor phase
d_z	total water body depth
EDS	Explosive Destruction System
ED_{dir}	exposure duration for direct pathways
$ED_{ind}(T_2)$	exposure duration for indirect pathways
EF	exposure frequency
EF_{dermal}	exposure frequency – dermal water
EIS	Environmental Impact Statement
EPI	Estimation Program Interface
ER	soil enrichment ratio
ET	exposure time
E_v	average annual evapo-transpiration
EV_{dermal}	event frequency - dermal water
F	fraction of plant grown on contaminated soil
f_1	fraction of ingested chemical that is stored in fat
f_2	fraction of mother's weight that is fat
f_3	fraction of fat in breast milk
f_4	fraction of ingested chemical which is absorbed
f_{pl}	fraction of chemical that is stored in the blood plasma
F_{beef}	fraction of consumed beef that is contaminated
F_{chick}	fraction of consumed chicken that is contaminated

Acronym/ Abbreviation	Definition
F_{egg}	fraction of consumed eggs that are contaminated
f_{fd}	fraction of chemical that is freely dissolved in water
F_{fish}	fraction of consumed fish that is contaminated
F_{milk}	fraction of consumed dairy milk that is contaminated
$f_{oc,bs}$	fraction of organic carbon in bottoms sediment
$f_{oc,s}$	fraction of organic carbon in soils
$f_{oc,sw}$	fraction of organic carbon in suspended sediments
F_p	fraction of consumed produce that is contaminated
f_{pm}	fraction of mother's weight that is blood plasma
F_{pork}	fraction of consumed pork that is contaminated
F_{soil}	fraction of consumed soil that is contaminated
ft^3	cubic foot
ft^3/s	cubic feet per second
F_v	fraction of air concentration in vapor phase
F_w	fraction of wet deposition that adheres to plant
f_{water}	fraction of forage that is water
g	gram(s)
h	half-life of chemical in adults
H	Henry's Law constant
HHRAP	Human Health Risk Assessment Protocol
HI	hazard index
I	Average annual irrigation
inch/yr	inch(es) per year
IR	Inhalation rate
IR_{milk}	ingestion rate of breast milk
ISC3	Industrial Source Complex
k	von Karman's constant
K	USLE erodibility factor
K_{ca}	cuticle-air partition coefficient
K_{cw}	cuticle-water partition coefficient
Kd_{bs}	bed sediment/sediment pore water partition coefficient
Kd_s	soil-water partition coefficient
Kd_{sw}	suspended sediment/surface water partition coefficient
K_{oc}	organic carbon-water partition coefficient
K_{ow}	octanol-water partition coefficient

Acronym/ Abbreviation	Definition
kg	kilogram(s)
kp	plant surface loss coefficient
K_p	dermal permeability coefficient of chemical in water
kse	loss constant due to erosion
ksg	loss constant due to degradation
K_{ow}	octanol-water partition coefficient
LS	USLE length-slope factor
l_{sc}	thickness of stratum corneum
m	average maternal intake of chemical
m	meter(s)
m^2	square meter(s)
m^3/yr	cubic meter(s) per year
MF	metabolism factor
mg	milligram(s)
MPHRA	Multiple Pathway Health Risk Assessment
MW	molecular weight
NCDC	National Climatic Data Center
NOAA	National Oceanic & Atmospheric Administration
NRCS	Natural Resources Conservation Service
P	average annual precipitation
Pa	Pascal
P_{ca}	gaseous phase permeance coefficient
PCAPP	Pueblo Chemical Agent-Destruction Pilot Plant
PCD	Pueblo Chemical Depot
$P_{C_{bm}}$	partition coefficient for chemical between plasma and breast milk aqueous phase
P_{cw}	aqueous phase permeance coefficient
PF	USLE supporting practice factor
POC	particulate organic carbon
Q	stack emission rate
$Qp_{forage(beef)}$	beef cattle consumption rate of forage
$Qp_{forage(chicken)}$	chicken consumption rate of forage
$Qp_{forage(dairy)}$	dairy cattle consumption rate of forage
$Qp_{forage(pork)}$	swine consumption rate of forage
$Qp_{grain(beef)}$	beef cattle consumption rate of grain

Acronym/ Abbreviation	Definition
$Qp_{grain(chicken)}$	chicken consumption rate of grain
$Qp_{grain(dairy)}$	dairy cattle consumption rate of grain
$Qp_{grain(pork)}$	swine consumption rate of grain
$Qp_{silage(beef)}$	beef cattle consumption rate of silage
$Qp_{silage(chicken)}$	chicken consumption rate of silage
$Qp_{silage(dairy)}$	dairy cattle consumption rate of silage
$Qp_{silage(pork)}$	swine consumption rate of silage
Qs_{beef}	beef cattle consumption rate of soil
$Qs_{chicken}$	chicken consumption rate of soil
Qs_{dairy}	dairy cattle consumption rate of soil
Qs_{pork}	swine consumption rate of soil
R	universal gas constant
RAGS	Risk Assessment Guidance for Superfund
RCF	root concentration factor
r_{cl}	cuticular resistance for individual leaves to uptake by lipids
RF	USLE rainfall (or erosivity) factor
RO	average annual runoff
Rp	interception fraction of edible portion of plant
Rp_{forage}	interception fraction of edible portion of plant for forage
Rp_{silage}	interception fraction of edible portion of plant for silage
RUSLE2	Revised Universal Soil Loss Equation Soil Erosion Prediction Program, Version 2
SA	skin surface area available for contact
S_T	Whitby's average surface area of particulates
t^*	time to reach steady-state
$t_{1/2}$	COPC half life in soil
T_a	ambient air temperature
tD	total time period over which deposition occurs
t_{event}	duration of swimming event
Tp	length of plant exposure to deposition of edible portion of plant, per harvest
Tp_{forage}	length of plant exposure to deposition of edible portion of plant for forage, per harvest
Tp_{silage}	length of plant exposure to deposition of edible portion of plant for silage, per harvest
TSS	total suspended solids

Acronym/ Abbreviation	Definition
T_{wk}	water body temperature
US	United States
US Army	United States Army
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
USLE	Universal Soil Loss Equation
Vf_x	average volumetric flow rate through water body
VG_{ag}	above-ground fruit/vegetable correction factor
VG_{forage}	forage correction factor
VG_{silage}	silage correction factor
V_m	molar volume of the liquid chemical at the normal boiling point
V_p	vapor pressure
W	wind speed
Yp	yield or standing crop biomass of edible portion of plant
Yp_{forage}	yield or standing crop biomass of edible portion of plant for forage
Yp_{silage}	yield or standing crop biomass of edible portion of plant for silage
Z_s	soil mixing depth

F SUMMARY OF DATA SOURCES FOR PARAMETERS USED IN THE MULTIPLE PATHWAY HEALTH RISK ASSESSMENT

Five different types of parameter values are used throughout the Multiple Pathway Health Risk Assessment (MPHRA). These parameter types are:

- Modeled values: parameter values that are the direct outputs from the air dispersion modeling and are discussed in Section 3.
- Default values: parameter values recommended by guidance documents for use when site- or chemical-specific data are unavailable.
- Site-specific values: parameter values that are specific to the Pueblo Chemical Depot (PCD), such as average annual precipitation, water body surface area, and the total watershed area receiving chemical deposition.
- Exposure scenario-specific values: parameters that vary between the different exposure scenarios evaluated under this MPHRA and include such items as the body weight of an individual, the exposure duration of the scenario, etc.
- Chemical-specific values: parameters that have values specific to each chemical of potential concern (COPC) such as physical, chemical, and transport properties.

Table F-1 categorizes each value used in the MPHRA as a modeled, site-specific, chemical-specific, exposure scenario-specific, or default parameter.

Table F-1. Parameters Used in the MPHRA

Parameter	Variable	Parameter Type
Above-ground fruit/vegetable correction factor	VG_{aq}	Chemical-specific
Air-to-plant biotransfer factor	BV_{aq}	Chemical-specific
Ambient air temperature	T_a	Default
Average annual evapo-transpiration	E_v	Site-specific
Average annual irrigation	I	Site-specific
Average annual precipitation	P	Site-specific
Average annual runoff	RO	Site-specific
Average maternal intake of chemical	m	Chemical-specific
Average volumetric flow rate through water body	Vf_x	Site-specific
Averaging time for carcinogenic effects	AT_{carc}	Exposure scenario-specific
Averaging time for noncarcinogenic direct pathways	$AT_{non\ carc,\ direct}$	Exposure scenario-specific
Averaging time for noncarcinogenic indirect pathways	$AT_{noncarc,\ indirect}$	Exposure scenario-specific
Bed sediment concentration	C_{BS}	Default
Bed sediment porosity	θ_{ps}	Default
Bed sediment/sediment pore water partition coefficient	Kd_{bs}	Chemical-specific
Beef cattle consumption rate of forage	$Qp_{forage(beef)}$	Default
Beef cattle consumption rate of grain	$Qp_{grain(beef)}$	Default
Beef cattle consumption rate of silage	$Qp_{silage(beef)}$	Default
Beef cattle consumption rate of soil	Qs_{beef}	Default
Bioaccumulation factor	BAF_{fish}	Chemical-specific
Bioconcentration factor	BCF_{fish}	Chemical-specific
Biota-to-sediment accumulation factor	$BSAF_{fish}$	Chemical-specific
Biotransfer factor for beef	Ba_{beef}	Chemical-specific
Biotransfer factor for chicken	Ba_{chick}	Chemical-specific
Biotransfer factor for eggs	Ba_{egg}	Chemical-specific
Biotransfer factor for milk	Ba_{milk}	Chemical-specific
Biotransfer factor for pork	Ba_{pork}	Chemical-specific

Table F-1. Parameters Used in the MPHRA (continued)

Parameter	Variable	Parameter Type
Body surface area	A	Exposure scenario-specific
Body weight	BW	Exposure scenario-specific
Chicken consumption rate of forage	$Qp_{forage(chicken)}$	Default
Chicken consumption rate of grain	$Qp_{grain(chicken)}$	Default
Chicken consumption rate of silage	$Qp_{silage(chicken)}$	Default
Chicken consumption rate of soil	$Qs_{chicken}$	Default
Consumption rate of beef	CR_{beef}	Exposure scenario-specific
Consumption rate of below-ground vegetables	CR_{bg}	Exposure scenario-specific
Consumption rate of chicken	CR_{chick}	Exposure scenario-specific
Consumption rate of eggs	CR_{egg}	Exposure scenario-specific
Consumption rate of exposed fruit	$CR_{exposed\ fruit}$	Exposure scenario-specific
Consumption rate of exposed vegetables	$CR_{exposed\ veg}$	Exposure scenario-specific
Consumption rate of fish	CR_{fish}	Exposure scenario-specific
Consumption rate of milk	CR_{milk}	Exposure scenario-specific
Consumption rate of pork	CR_{pork}	Exposure scenario-specific
Consumption rate of protected fruit	$CR_{protected\ fruit}$	Exposure scenario-specific
Consumption rate of protected vegetables	$CR_{protected\ veg}$	Exposure scenario-specific
Consumption rate of soil	CR_{soil}	Exposure scenario-specific
Cuticular resistance for individual leaves to uptake by lipids	r_{cl}	Chemical-specific
Dairy cattle consumption rate of forage	$Qp_{forage(dairy)}$	Default
Dairy cattle consumption rate of grain	$Qp_{grain(dairy)}$	Default
Dairy cattle consumption rate of silage	$Qp_{silage(dairy)}$	Default
Dairy cattle consumption rate of soil	Qs_{dairy}	Default
Density of air	ρ_a	Default
Density of water	ρ_w	Default
Depth of upper benthic layer	d_{bs}	Default
Depth of water column	d_{wc}	Site-specific
Dermal absorption fraction	ABS_d	Chemical-specific
Dermal permeability coefficient of chemical in water	Kp	Chemical-specific
Diffusivity of chemical in air	D_a	Chemical-specific
Diffusivity of chemical in water	D_w	Chemical-specific
Dimensionless viscous sublayer thickness	λ_z	Default
Drag coefficient	C_d	Default
Duration of swimming event	t_{event}	Site-specific
Empirical intercept coefficient	a	Default
Empirical slope coefficient	b	Default
Event frequency - dermal water	EV_{dermal}	Exposure scenario-specific
Exposure duration for direct pathways	ED_{dir}	Exposure scenario-specific
Exposure duration for indirect pathways	$Ed_{ind} (T_2)$	Exposure scenario-specific
Exposure frequency – dermal water	EF_{dermal}	Exposure scenario-specific
Exposure frequency	EF	Exposure scenario-specific
Exposure time	ET	Exposure scenario-specific
Forage correction factor	VG_{forage}	Default
Fraction of air concentration in vapor phase	F_v	Chemical-specific
Fraction of chemical that is stored in fat	f_1	Chemical-specific
Fraction of chemical that is stored in the blood plasma	f_2	Chemical-specific
Fraction of contaminant absorbed in the gastrointestinal tract	ABS_{GI}	Chemical-specific
Fraction of consumed beef that is contaminated	F_{beef}	Exposure scenario-specific
Fraction of consumed chicken that is contaminated	F_{chick}	Exposure scenario-specific
Fraction of consumed dairy milk that is contaminated	F_{milk}	Exposure scenario-specific
Fraction of consumed eggs that are contaminated	F_{egg}	Exposure scenario-specific
Fraction of consumed fish that is contaminated	F_{fish}	Exposure scenario-specific
Fraction of consumed pork that is contaminated	F_{pork}	Exposure scenario-specific
Fraction of consumed produce that is contaminated	F_p	Exposure scenario-specific
Fraction of consumed soil that is contaminated	F_{soil}	Exposure scenario-specific
Fraction of fat in breast milk	f_3	Default
Fraction of ingested chemical which is absorbed	f_4	Chemical-specific
Fraction of mother's weight that is blood plasma	f_{pm}	Default
Fraction of mother's weight that is fat	f_2	Default
Fraction of plant that is grown on contaminated soil	F	Default
Fraction of wet deposition that adheres to plant	F_w	Default
Half-life of chemical in adults	h	Chemical-specific

Table F-1. Parameters Used in the MPHRA (continued)

Parameter	Variable	Parameter Type
Henry's Law constant	H	Chemical-specific
Impervious watershed area receiving chemical deposition	A_I	Site-specific
Incidental consumption rate of surface water	CR_{sw}	Exposure scenario-specific
Ingestion rate of breast milk	IR_{milk}	Exposure scenario-specific
Inhalation rate	IR	Exposure scenario-specific
Interception fraction of edible portion of plant	R_p	Default
Interception fraction of edible portion of plant for forage	$R_{p_{forage}}$	Default
Interception fraction of edible portion of plant for silage	$R_{p_{silage}}$	Default
Length of plant exposure to deposition per of edible portion of plant, per harvest	T_p	Default
Length of plant exposure to deposition of edible portion of plant for forage, per harvest	$T_{p_{forage}}$	Default
Length of plant exposure to deposition of edible portion of plant for silage, per harvest	$T_{p_{silage}}$	Default
Loss constant due to degradation	k_{sg}	Chemical-specific
Loss constant due to erosion	k_{se}	Default
Metabolism factor	MF	Chemical-specific
Molecular weight	MW	Chemical-specific
Octanol-water partition coefficient	K_{ow}	Chemical-specific
Particle phase air concentration	C_{yp}	Modeled
Partition coefficient for chemical between plasma and breast milk aqueous phase	$P_{c_{bm}}$	Default
Plant surface loss coefficient	k_p	Default
Plant-to-soil bioconcentration factor for above-ground produce	Br_{ag}	Chemical-specific
Root concentration factor	RCF	Chemical-specific
Silage correction factor	VG_{silage}	Default
Skin surface area available for contact	SA	Exposure scenario-specific
Soil adherence factor	AF	Exposure scenario-specific
Soil bioavailability factor	B_s	Default
Soil bulk density	BD	Default
Soil enrichment ratio	ER	Default
Soil mixing depth	Z_s	Default
Soil volumetric water content	θ_{sw}	Default
Soil-water partition coefficient	Kd_s	Chemical-specific
Solids particulate density	ρ_{soil}	Default
Stack emission rate	Q	Modeled
Suspended sediment/surface water partition coefficient	Kd_{sw}	Chemical-specific
Swimming frequency	$F_s (t_{event})$	Exposure scenario-specific
Swine consumption rate of forage	$Q_{p_{forage}(pork)}$	Default
Swine consumption rate of grain	$Q_{p_{grain}(pork)}$	Default
Swine consumption rate of silage	$Q_{p_{silage}(pork)}$	Default
Swine consumption rate of soil	$Q_{S_{pork}}$	Default
Temperature correction factor	θ	Default
Thickness of stratum corneum	l_{sc}	Default
Time period over which deposition occurs	tD	Site-specific
Total suspended solids	TSS	Default
Total water body depth	d_z	Site-specific
Total watershed area receiving chemical deposition	A_L	Site-specific
Universal gas constant	R	Default
USLE cover management factor	C	Default
USLE erodibility factor	K	Site-specific
USLE length-slope factor	LS	Default
USLE rainfall (or erosivity) factor	RF	Site-specific
USLE supporting practice factor	PF	Default
Vapor phase air concentration	C_{yv}	Modeled
Vapor pressure	V_p	Chemical-specific
Viscosity of air corresponding to air temperature	μ_a	Default
Viscosity of water corresponding to water temperature	μ_w	Default
von Karman's constant	k	Default
Water body surface area	A_w	Site-specific
Water body temperature	T_{wk}	Default
Watershed vapor phase air concentration	C_{ywv}	Modeled

Table F-1. Parameters Used in the MPHRA (continued)

Parameter	Variable	Parameter Type
Wind speed	W	Default
Yearly dry deposition from particle phase	$Dydp$	Modeled
Yearly dry deposition from vapor phase	$Dydv$	Modeled
Yearly watershed dry deposition from particle phase	$Dywdp$	Modeled
Yearly watershed dry deposition from vapor phase	$Dywdv$	Modeled
Yearly watershed wet deposition from particle phase	$Dywwp$	Modeled
Yearly watershed wet deposition from vapor phase	$Dywwv$	Modeled
Yearly wet deposition from particle phase	$Dywp$	Modeled
Yearly wet deposition from vapor phase	$Dywv$	Modeled
Yield or standing crop biomass of edible portion of plant	Yp	Default
Yield or standing crop biomass of edible portion of plant for forage	Yp_{forage}	Default
Yield or standing crop biomass of edible portion of plant for silage	Yp_{silage}	Default

F.1 DEFAULT VALUES

Default values used in this MPHRA are recommended for use by guidance documents (United States Environmental Protection Agency [USEPA], 2005; USEPA, 2004) when reliable site-specific or chemical-specific data are unavailable. Table F-2 presents default values used in the MPHRA.

Table F-2. Default Values Used in the MPHRA^a

Parameter	Variable	Value	Units
Ambient air temperature	T_a	298	K
Bed sediment concentration	C_{BS}	1	g/cm ³
Bed sediment porosity	θ_{bs}	0.6	$\ell_{water}/\ell_{sediment}$
Beef cattle consumption rate of forage	$Qp_{forage}(beef)$	8.8	kg/day
Beef cattle consumption rate of grain	$Qp_{grain}(beef)$	0.47	kg/day
Beef cattle consumption rate of silage	$Qp_{silage}(beef)$	2.5	kg/day
Beef cattle consumption rate of soil	QS_{beef}	0.5	kg/day
Chicken consumption rate of forage	$Qp_{forage}(chicken)$	0	kg/day
Chicken consumption rate of grain	$Qp_{grain}(chicken)$	0.2	kg/day
Chicken consumption rate of silage	$Qp_{silage}(chicken)$	0	kg/day
Chicken consumption rate of soil	$QS_{chicken}$	0.022	kg/day
Dairy cattle consumption rate of forage	$Qp_{forage}(dairy)$	13.2	kg/day
Dairy cattle consumption rate of grain	$Qp_{grain}(dairy)$	3	kg/day
Dairy cattle consumption rate of silage	$Qp_{silage}(dairy)$	4.1	kg/day
Dairy cattle consumption rate of soil	QS_{dairy}	0.4	kg/day
Density of air	ρ_a	0.0012	g/cm ³
Density of water	ρ_w	1	g/cm ³
Depth of upper benthic layer	d_{bs}	0.03	m
Dimensionless viscous sublayer thickness	λ_z	4	dimensionless
Drag coefficient	Cd	0.0011	dimensionless
Empirical intercept coefficient	a	1.9	dimensionless
Empirical slope coefficient	b	0.125	dimensionless
Forage correction factor	VG_{forage}	1	dimensionless
Fraction of fat in breast milk	f_3	0.04 ^b	dimensionless ^b
Fraction of mother's weight that is blood plasma	f_{pm}	0.046 ^b	dimensionless ^b
Fraction of mother's weight that is fat	f_2	0.3 ^b	dimensionless ^b
Fraction of plant that is grown on contaminated soil	F	1	dimensionless
Fraction of wet deposition that adheres to plant	F_w	0.6	dimensionless
Interception fraction of edible portion of plant	Rp	0.39	dimensionless
Interception fraction of edible portion of plant for forage	Rp_{forage}	0.5	dimensionless
Interception fraction of edible portion of plant for silage	Rp_{silage}	0.46	dimensionless
Length of plant exposure to deposition of edible portion of plant, per harvest	Tp	0.16	yr
Length of plant exposure to deposition of edible portion of plant for forage, per harvest	Tp_{forage}	0.12	yr
Length of plant exposure to deposition of edible portion of plant for silage, per harvest	Tp_{silage}	0.16	yr

Table F-2. Default Values Used in the MPHRA (continued)^a

Parameter	Variable	Value	Units
Loss constant due to erosion	k_{se}	0	yr ⁻¹
Partition coefficient for chemical between plasma and breast milk aqueous phase	$P_{C_{bm}}$	1 ^b	dimensionless ^b
Plant surface loss coefficient	k_p	18	yr ⁻¹
Silage correction factor	VG_{silage}	0.5	dimensionless
Soil bioavailability factor	B_s	1	dimensionless
Soil bulk density	BD	1.5	g soil/cm ³ soil
Soil enrichment ratio	ER	3	dimensionless
Soil mixing depth	Z_s	2	cm
Soil volumetric water content	θ_{sw}	0.2	m ³ water/cm ³
Solids particulate density	ρ_{soil}	2.7	g/cm ³
Swine consumption rate of forage	$Q_{p_{forage(pork)}}$	0	kg/day
Swine consumption rate of grain	$Q_{p_{grain(pork)}}$	3.3	kg/day
Swine consumption rate of silage	$Q_{p_{silage(pork)}}$	1.4	kg/day
Swine consumption rate of soil	$Q_{s_{pork}}$	0.37	kg/day
Temperature correction factor	θ	1.026	dimensionless
Thickness of stratum corneum	l_{sc}	0.001 ^b	cm ^b
Total suspended solids	TSS	10	mg/l
Universal gas constant	R	8.205 x 10 ⁻⁵	atm-m ³ /mol-K
USLE cover management factor	C	0.1	dimensionless
USLE length-slope factor	LS	1.5	dimensionless
USLE supporting practice factor	PF	1	dimensionless
Viscosity of air corresponding to air temperature	μ_a	0.000181	g/cm-s
Viscosity of water corresponding to water temperature	μ_w	0.0169	g/cm-s
von Karman's constant	k	0.4	dimensionless
Water body temperature	T_{wk}	298	K
Wind speed	W	3.9	m/s
Yield or standing crop biomass of edible portion of plant	Y_p	2.24	kg dry weight/m ²
Yield or standing crop biomass of edible portion of plant for forage	$Y_{p_{forage}}$	0.24	kg dry weight/m ²
Yield or standing crop biomass of edible portion of plant for silage	$Y_{p_{silage}}$	0.8	kg dry weight/m ²

- a. USEPA, 2005. *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*. Office of Solid Waste and Emergency Response, Washington, DC. EPA530-R-05-006, September 2005.
- b. USEPA, 2004. *Risk Assessment Guidance for Superfund Volume 1: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*. Office of Solid Waste and Emergency Response, Washington, DC. EPA/540/R/99/005, July 2004.

F.2 SITE-SPECIFIC VALUES

Table F-3 presents site-specific values used in this MPHRA. Additional discussion of the sources of each of the site-specific values is provided in the following subsections.

F.2.1 Average Annual Evapo-transpiration

Evapo-transpiration is the sum of the water released through evaporation and the water released through plant leaves via transpiration. Two reference sources for evaporation in Pueblo, Colorado, were acquired; however, no reference sources were found that provided evapo-transpiration rates. A range between 46 and 50 inches per year (inch/yr) of evaporation was found from maps contained in the *Water Atlas of the United States: Basic Facts about the Nation's Water Resources* (Miller, 1963). Another reference source (Chafin, 1996) provided a value of 48 inches/yr of evaporation in Pueblo, Colorado. In the MPHRA, 48 inches/yr (121.9 centimeter per year (cm/yr)) was used as the rate of evapo-transpiration.

F.2.2 Average Annual Irrigation

Site-specific data indicate that the area immediately surrounding PCD is not irrigated. The average annual irrigation was set to 0 inch/yr (0 cm/yr) to reflect this lack of irrigation.

Table F-3. Site-specific Values Used in the MPHRA

Parameter	Variable	Value	Units
Average annual evapo-transpiration	E_v	121.9	cm/yr
Average annual irrigation	I	0	cm/yr
Average annual precipitation	P	31.5	cm/yr
Average annual runoff	RO	1.27	cm/yr
Average volumetric flow rate through water body	Vf_x	2,680,560	m ³ /yr
Depth of water column	d_{wc}	5	m
Duration of swimming event	t_{event}	3	hour
Impervious watershed area receiving chemical deposition	A_i	3,670,320	m ²
Time period over which deposition occurs	tD	5	yr
Total water body depth	d_z	5.03	m
Total watershed area receiving chemical deposition	A_L	183,516,000	m ²
USLE erodibility factor	K	0.37	ton/acre
USLE rainfall factor	RF	31	yr ⁻¹
Water body surface area	A_w	75,000	m ²

F.2.3 Average Annual Precipitation

The average annual precipitation for Pueblo, Colorado, was obtained from the National Oceanic & Atmospheric Administration (NOAA, 2004) National Climatic Data Center (NCDC) for station number 144 Pueblo AP located at the Pueblo Memorial Airport. NCDC provides normal yearly climatic data for station number 144 Pueblo AP for the period 1971 through 2000. For this time period, the normal yearly precipitation in Pueblo, Colorado was 12.39 inches/yr (31.5 cm/yr).

F.2.4 Average Annual Runoff

The average annual runoff for Pueblo, Colorado, was obtained from the *Water Atlas of the United States: Basic Facts about the Nation's Water Resources* (Miller, 1963). Maps contained within this reference show lines of constant runoff. Pueblo, Colorado, is located in an area with average annual runoff of less than 1 inch per year. A value of 0.5 inch/yr (1.27 cm/yr) was used as an estimate of the average annual runoff

F.2.5 Average Volumetric Flow Rate of Water body

Volumetric flow rates for the water bodies located closest to the area of maximum modeled impacts were not available. Data were available in the Environmental Impact Statement (EIS) for Pueblo Chemical Agent-Destruction Pilot Plant (PCAPP) (United States [US] Army, 2002) for Chico Creek, a creek on the western edge of PCD of similar size to the creek that feeds the water bodies. Flow in these creeks is intermittent (i.e., when there is no rainfall, there is little to no water flowing in them). Data for Chico Creek indicated a maximum flow rate of 330 cubic feet per second (ft³/s) with an average flow rate of 3 ft³/s. Approximately 31 percent of the time, there was less than 0.1 ft³/s flowing through the creek. The average value of 3 ft³/s was converted to cubic meters per year (m³/yr), resulting in the volumetric flow rate of the water body of 2,680,560 m³/yr used in the MPHRA.

F.2.6 Depth of the Water Column and Total Water Body Depth

The depth of the water column in the water body located just north of PCD was estimated. A water column depth of 5 meters (m) was used for Thatcher Reservoir. The total water body depth was calculated by adding the default value for the benthic sediment layer of 0.03 m to the water column depth, resulting in a total water body depth of 5.03 m used in the MPHRA.

F.2.7 Duration of Swimming Event

The length of swimming events in subject water body was determined to be 3 hours per event based upon conversations with the owner of the water body.

F.2.8 Water Body, Impervious Watershed, and Total Watershed Areas Receiving Chemical Deposition

The water body and watershed areas were obtained by examining the North Avondale United State Geological Survey (USGS) 7.5-minute quadrangle map. The total water body area of Thatcher Reservoir was determined to be 75,000 square meters (m²) directly from the topographic map. The total watershed area is 183,516,00 m² as reported by USGS for the Upper Haynes Creek watershed (HUC C-12 110200050103). The impervious watershed area was determined by examining aerial photographs of the region as well as the topographical map. The total watershed area has few impervious structures other than the U.S. DOT Transportation Technology Center and Thatcher's residence. The impervious watershed area was conservatively estimated to be 2 percent of the total watershed area, or 3,670,320 m².

F.2.9 Time Period Over Which Deposition Occurs

The time period over which deposition occurs is equal to the total duration of PCAPP and Explosive Destruction System (EDS) emissions (i.e., the total operating life of PCAPP). For this MPHRA, a total of 5 years was used for the duration of PCAPP hazardous waste operations.

F.2.10 USLE Rainfall and Erodibility Factors

The universal soil loss equation (USLE) rainfall factor was obtained from the Revised Universal Soil Loss Equation Soil Erosion Prediction Program, Version 2 (RUSLE2) provided by the Natural Resources Conservation Service (NRCS, 2006). A database of climatic data for the State of Colorado was imported into RUSLE2 to determine the value of the rainfall factor, or erosivity. Values in the database were provided on a county-by-county basis for different annual precipitation values. For 13 inches of precipitation per year in Pueblo County, the USLE rainfall factor was determined to be 31 year⁻¹.

A database containing soil information for Pueblo County was imported into RUSLE2 to determine the USLE erodibility factor for PCD. Erodibility values were obtained for Valent, Olney, Vona, Arvada, Keyner, Limon, Razor, Midway, Stoneham, Adena, Manzanola, Las Anima, Glenberg, and Apishapa soil types. These soil types were selected based on the list of soil types identified in the EIS for PCAPP (US Army, 2002). The erodibility factors for these soil types ranged from 0.15 to 0.37 ton per acre. Since higher erodibility factors are more conservative in this analysis, the high end of the erodibility range, 0.37 ton per acre, was used as the USLE erodibility factor in the MPHRA.

F.3 EXPOSURE SCENARIO-SPECIFIC VALUES

Tables F-4 through F-6 present the exposure scenario-specific values used in each of the exposure scenarios evaluated in the MPHRA.

F.4 CHEMICAL-SPECIFIC VALUES

The following sections present and discuss the source of and, if necessary, the derivation of each chemical-specific value used in this MPHRA.

F.4.1 Chemical and Physical Properties of COPCs

Table F-7 presents physical and chemical properties for all COPCs identified in the MPHRA obtained from various sources and used to evaluate overall excess lifetime cancer risk and hazard indices (HIs) for each exposure scenario. Generally, data were obtained from the Companion Database to the Human Health Risk Assessment Protocol (HHRAP) (USEPA, 2005). When data were unavailable in the Companion Database, other resources were used (and are identified in Table F-7) to find these factors. The following sections discuss procedures used when parameters in Table F-7 were derived using methods identified in Appendix A-2 of the HHRAP (USEPA, 2005).

Soil Loss Constant Due to Degradation. When available, the soil loss constant due to degradation was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). When degradation rates were unavailable from the Companion Database, half-lives of COPCs in soil were obtained from *The Handbook of Environmental Degradation Rates* (Howard et al., 1991) and the soil loss constant due to degradation was estimated using Equation A-2-13 from the HHRAP (USEPA, 2005) (reproduced as Equation F-1 below):

$$k_{sg} = \frac{0.693}{t_{1/2}} \quad \text{Eq. F-1}$$

where

$$\begin{aligned} k_{sg} &= \text{loss constant due to degradation (yr}^{-1}\text{)} \\ t_{1/2} &= \text{chemical half-life in soil (yr)} \end{aligned}$$

When a soil loss constant due to degradation was not available from either source, the soil loss constant due to degradation was assigned a value of zero as a conservative assumption that none of the COPC is lost from soil due to biotic and abiotic degradation.

Log of the Octanol-Water Partition Coefficient. Several sources were used to obtain the log of the octanol-water partition coefficient, $\log K_{ow}$, for each COPC. When available, $\log K_{ow}$ was obtained from the Companion Database to the HHRAP (USEPA, 2005). In instances where the Companion Database did not contain values, $\log K_{ow}$ was obtained either from the PHYSPROP Database (Syracuse Research Corporation, 2003a) (Copyright © 1999 Syracuse Research Corporation) or the Estimation Program Interface (EPI) Suite (USEPA, 2000-2007) (Copyright © 2000-2007 USEPA).

Table F-4. Adult Exposure Scenario-specific Parameters^a

Parameter	Variable	Adult Resident	Adult Subsistence Fisher	Adult Subsistence Farmer	Adult Worker
Averaging time for carcinogenic effects (yr)	AT_{carc}	78	78	78	78
Averaging time for noncarcinogenic direct pathways (yr)	$AT_{noncarc, direct}$	5	5	5	5
Averaging time for noncarcinogenic indirect pathways (yr)	$AT_{noncarc, indirect}$	30	30	40	25
Body surface area exposed during swimming (cm ²)	SA	18,000 ^b	18,000 ^b	18,000 ^b	18,000 ^b
Body surface area exposed to soil (cm ²)	SA	5,700 ^b	5,700 ^b	5,700 ^b	3,330 ^b
Body weight (kg)	BW	80	80	80	80
Event frequency – dermal water (event/day)	EV_{dermal}	1 ^b	1 ^b	1 ^b	1 ^b
Exposure duration for direct pathways (yr)	ED_{dir}	5	5	5	5
Exposure duration for indirect pathways (yr)	$ED_{ind} (T_2)$	30	30	40	25 ^c
Exposure frequency (day/yr)	EF	350	350	350	250 ^c
Exposure frequency – dermal water (day/yr)	EF_{dermal}	12 ^d	12 ^d	12 ^d	n/a ^d
Exposure time (hr/day)	ET	24	24	24	8 ^c
Consumption rate:					
soil (kg/day)	CR_{soil}	0.0001	0.0001	0.0001	0.0001 ^c
exposed fruit (kg/day)	$CR_{exposed\ fruit}$	0.560	0.560	0.560	n/a
protected fruit (kg/day)	$CR_{protected\ fruit}$	0.648	0.648	0.648	n/a
exposed vegetables (kg/day)	$CR_{exposed\ veg}$	0.352	0.352	0.352	n/a
protected vegetables (kg/day)	$CR_{protected\ veg}$	0.248	0.248	0.248	n/a
below-ground vegetables (kg/day)	CR_{bg}	0.328	0.328	0.328	n/a
beef (kg/day)	CR_{beef}	0.157	0.157	0.157	n/a
pork (kg/day)	CR_{pork}	0.073	0.073	0.073	n/a
chicken (kg/day)	CR_{chick}	0.124	0.124	0.124	n/a
eggs (kg/day)	CR_{egg}	0.070	0.070	0.070	n/a
dairy milk (kg/day)	CR_{milk}	0.993	0.993	0.993	n/a
fish (kg/day)	CR_{fish}	0.168	0.168	0.168	n/a
incidental surface water (m ^l /hr)	CR_{sw}	71 ^c	71 ^c	71 ^c	n/a
breast milk (kg/day)	IR_{milk}	n/a	n/a	n/a	n/a
Inhalation rate (m ³ /hr)	IR	0.83	0.83	0.83	0.83
Soil fraction contaminated (dimensionless)	F_{soil}	1	1	1	1
Produce fraction contaminated (dimensionless)	F_p	0.4 ^e	0.4 ^e	1	n/a
Beef fraction contaminated (dimensionless)	F_{beef}	0.4 ^e	0.4 ^e	1	n/a
Pork fraction contaminated (dimensionless)	F_{pork}	0.4 ^e	0.4 ^e	1	n/a
Chicken fraction contaminated (dimensionless)	F_{chick}	0.4 ^e	0.4 ^e	1	n/a
Egg fraction contaminated (dimensionless)	F_{egg}	0.4	0.4	1	n/a
Milk fraction contaminated (dimensionless)	F_{milk}	0.4 ^e	0.4 ^e	1	n/a
Fish fraction contaminated (dimensionless)	F_{fish}	0.4 ^e	1	0.4 ^e	n/a
Soil adherence factor (mg/cm ² -event)	AF	0.07 ^b	0.07 ^b	0.07 ^b	0.20 ^b
Duration of swimming event (hr/day)	t_{event}	3 ^d	3 ^d	3 ^d	n/a ^d

- a. USEPA, 2011. *Exposure Factors Handbook*. EPA/600/R-09/052F, September 2011.
 - b. USEPA, 2004. *Risk Assessment Guidance for Superfund Volume 1: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*. Office of Solid Waste and Emergency Response, Washington, DC. EPA/540/R/99/005, July 2004.
 - c. US Environmental Protection Agency, 2004, *Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*, Office of Superfund Remediation and Technology Innovation, Washington, DC. EPA/540/R/99/005.
 - d. Information obtained from the owner of the impacted water body.
 - e. As a conservative approach in this HRA, residents will obtain 40 percent of their produce, beef, milk, and pork from local subsistence farmers and 40 percent of their fish from local sources.
- n/a Pathway not evaluated for this human receptor.

Table F-5. Child Exposure Scenario-specific Parameters^a

Parameter	Variable	Child Resident	Child Subsistence Fisher	Child Subsistence Farmer
Averaging time for carcinogenic effects (yr)	AT_{carc}	78	78	78
Averaging time for noncarcinogenic direct pathways (yr)	$AT_{noncarc, direct}$	5	5	5
Averaging time for noncarcinogenic indirect pathways (yr)	$AT_{noncarc, indirect}$	5	5	5
Body surface area exposed during swimming (cm ²)	SA	6,600 ^b	6,600 ^b	6,600 ^b
Body surface area exposed to soil (cm ²)	SA	2,800 ^b	2,800 ^b	2,800 ^b
Body weight (kg)	BW	16.2	16.2	16.2
Event frequency – dermal water (event/day)	EV_{dermal}	1 ^b	1 ^b	1 ^b
Exposure duration for direct pathways (yr)	ED_{dir}	5	5	5
Exposure duration for indirect pathways (yr)	$ED_{ind} (T_2)$	5	5	5
Exposure frequency (day/yr)	EF	350	350	350
Exposure frequency – dermal water (day/yr)	EF_{dermal}	12 ^c	12 ^c	12 ^c
Exposure time (hr/day)	ET	24	24	24
Consumption rate:				
soil (kg/day)	CR_{soil}	0.0002	0.0002	0.0002
exposed fruit (kg/day)	$CR_{exposed fruit}$	0.469	0.469	0.469
protected fruit (kg/day)	$CR_{protected fruit}$	0.324	0.324	0.324
exposed vegetables (kg/day)	$CR_{exposed veg}$	0.118	0.118	0.118
protected vegetables (kg/day)	$CR_{protected veg}$	0.098	0.098	0.098
below-ground vegetables (kg/day)	CR_{bg}	0.123	0.123	0.123
beef (kg/day)	CR_{beef}	0.052	0.052	0.052
pork (kg/day)	CR_{pork}	0.024	0.024	0.024
chicken (kg/day)	CR_{chick}	0.047	0.047	0.047
eggs (kg/day)	CR_{egg}	0.032	0.032	0.032
milk (kg/day)	CR_{milk}	1.052	1.052	1.052
fish (kg/day)	CR_{fish}	0.067 ^d	0.067 ^d	0.067 ^d
incidental surface water (m ^l /hr)	CR_{sw}	120 ^e	120 ^e	120 ^e
breast milk (kg/day)	IR_{milk}	n/a	n/a	n/a
Soil fraction contaminated (dimensionless)	F_{soil}	1	1	1
Produce fraction contaminated (dimensionless)	F_p	0.4 ^f	0.4 ^f	1
Beef fraction contaminated (dimensionless)	F_{beef}	0.4 ^f	0.4 ^f	1
Pork fraction contaminated (dimensionless)	F_{pork}	0.4 ^f	0.4 ^f	1
Chicken fraction contaminated (dimensionless)	F_{chick}	0.4 ^f	0.4 ^f	1
Egg fraction contaminated (dimensionless)	F_{egg}	0.4 ^f	0.4 ^f	1
Milk fraction contaminated (dimensionless)	F_{milk}	0.4 ^f	0.4 ^f	1
Fish fraction contaminated (dimensionless)	F_{fish}	0.4 ^f	1	0.4 ^f
Soil adherence factor (mg/cm ² -event)	AF	0.20 ^b	0.20 ^b	0.20 ^b
Duration of swimming event (hr/day)	t_{event}	3 ^c	3 ^c	3 ^c

- USEPA, 2011. *Exposure Factors Handbook*. EPA/600/R-09/052F, September 2011.
- USEPA, 2004. *Risk Assessment Guidance for Superfund Volume 1: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*. Office of Solid Waste and Emergency Response, Washington, DC. EPA/540/R/99/005, July 2004.
- Information obtained from the owner of the impacted water body.
- USEPA, 2002. *Estimated Per Capita Fish Consumption in the United States*. Washington, DC. EPA-821-C-02-003, August, 2002.
- USEPA, 1989. *Risk Assessment Guidance for Superfund, Volume 1, Human Health Evaluation Manual (Part A)*. Interim Final. Office of Emergency and Remedial Response. EPA/504/1-89/002.
- As a conservative approach in this HRA, residents will obtain 40 percent of their produce, beef, milk, and pork from local subsistence farmers and 40 percent of their fish from local sources.

Table F-6. Infant Exposure Scenario-specific Parameters^a

Parameter	Variable	Infant Resident	Infant Subsistence Fisher	Infant Subsistence Farmer
Averaging time for carcinogenic effects (yr)	AT_{carc}	78	78	78
Averaging time for noncarcinogenic direct pathways (yr)	$AT_{noncarc, direct}$	1	1	1
Averaging time for noncarcinogenic indirect pathways (yr)	$AT_{noncarc, indirect}$	1	1	1
Body surface area exposed during swimming (cm ²)	SA	n/a	n/a	n/a
Body surface area exposed to soil (cm ²)	SA	2,625 ^b	2,625 ^b	2,625 ^b
Body weight (kg)	BW	7.8	7.8	7.8
Event frequency – dermal water (event/day)	EV_{dermal}	1 ^b	1 ^b	1 ^b
Exposure duration for direct pathways (yr)	ED_{dir}	1	1	1
Exposure duration for indirect pathways (yr)	$ED_{ind} (T_2)$	1	1	1
Exposure frequency (day/yr)	EF	350	350	350
Exposure frequency – dermal water (day/yr)	EF_{dermal}	n/a ^c	n/a ^c	n/a ^c
Exposure time (hr/day)	ET	24	24	24
Consumption rate:				
soil (kg/day)	CR_{soil}	0.0002	0.0002	0.0002
exposed fruit (kg/day)	$CR_{exposed fruit}$	0.303	0.303	0.303
protected fruit (kg/day)	$CR_{protected fruit}$	0.065	0.065	0.065
exposed vegetables (kg/day)	$CR_{exposed veg}$	0.058	0.058	0.058
protected vegetables (kg/day)	$CR_{protect veg}$	0.061	0.061	0.061
below-ground vegetables (kg/day)	CR_{bg}	0.075	0.075	0.075
beef (kg/day)	CR_{beef}	0.014	0.014	0.014
pork (kg/day)	CR_{pork}	0.005	0.005	0.005
chicken (kg/day)	CR_{chick}	0.023	0.023	0.023
eggs (kg/day)	CR_{eggs}	0.01	0.01	0.01
milk (kg/day)	CR_{milk}	0.38	0.38	0.38
fish (kg/day)	CR_{fish}	0.023 ^d	0.023 ^d	0.023 ^d
incidental surface water (m ^l /hr)	CR_{sw}	n/a	n/a	n/a
breast milk (kg/day)	IR_{milk}	1.16 ^d	1.16 ^d	1.16 ^d
Soil fraction contaminated (dimensionless)	F_{soil}	1	1	1
Produce fraction contaminated (dimensionless)	F_p	0.4 ^e	0.4 ^e	1
Beef fraction contaminated (dimensionless)	F_{beef}	0.4 ^e	0.4 ^e	1
Pork fraction contaminated (dimensionless)	F_{pork}	0.4 ^e	0.4 ^e	1
Chicken fraction contaminated (dimensionless)	F_{chick}	0.4 ^e	0.4 ^e	1
Egg fraction contaminated (dimensionless)	F_{egg}	0.4 ^e	0.4 ^e	1
Milk fraction contaminated (dimensionless)	F_{milk}	0.4 ^e	0.4 ^e	1
Fish fraction contaminated (dimensionless)	F_{fish}	0.4 ^e	1	0.4 ^e
Soil adherence factor (mg/cm ² -event)	AF	0.20 ^b	0.20 ^b	0.20 ^b
Duration of swimming event (hr/day)	t_{event}	n/a ^c	n/a ^c	n/a ^c

- a. USEPA, 2011. *Exposure Factors Handbook*. EPA/600/R-09/052F, September 2011.
 - b. USEPA, 2004. *Risk Assessment Guidance for Superfund Volume 1: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*. Office of Solid Waste and Emergency Response, Washington, DC. EPA/540/R/99/005, July 2004.
 - c. Information obtained from the owner of the impacted water body.
 - d. USEPA, 2002. *Estimated Per Capita Fish Consumption in the United States*. Washington, DC. EPA-821-C-02-003, August, 2002.
 - e. As a conservative approach in this HRA, residents will obtain 40 percent of their produce, beef, milk, and pork from local subsistence farmers and 40 percent of their fish from local sources.
- n/a Pathway not evaluated for this human receptor.

Table F-7. Chemical and Physical Properties^a

COPC	Molecular Weight	Loss Constant due to Degradation	Soil-Water Partition Coefficient	Bed Sediment/Sediment Pore Water Partition Coefficient	Suspended Sediment-Surface Water Partition Coefficient	Log Octanol-Water Partition Coefficient	Henry's Law Constant	Diffusivity of Chemical in Air	Diffusivity of Chemical in Water	Vapor Pressure	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^h
	(g/mol)	(yr ⁻¹)	(cm ³ water/g soil)	(cm ³ /g/kg)	(l/kg)	(dimensionless)	(atm-m ³ /mol)	(cm ² /s)	(cm ² /s)	(Pa)	(s/cm)
	MW	ksg	K _{d,s}	K _{d,bs}	K _{d,sw}	log K _{ow}	H	D _a	D _w	V _p	r _{cl}
1,1,1,2-tetrachloroethane	167.84	3.78	3	12.02	22.54	3.03	0.00242	0.071	0.0000079	1.60E+03	2.59E+04
1,1,1-trichloroethane	133.37	0.93	0.22	5.4	10.1	2.5	0.017	0.078	0.0000088	1.65E+04	8.15E+04
1,1,2,2-tetrachloroethane	167.85	5.75	0.19	3.16	5.93	2.4	0.00034	0.071	0.0000079	6.13E+02	4.95E+04
1,1-dichloroethane	98.96	1.64	0.06	2.14	4.01	1.8	0.0056	0.074	0.0000105	3.07E+04	1.16E+05
1,1-dichloroethene	98.96	1.41	0.12	2.6	4.88	2.1	0.026	0.09	0.0000104	8.05E+04	5.78E+04
1,2,3-trichlorobenzene	181.45	0	19.3	77.2	144.8	4.05	0.00125	0.001	0.00001	2.80E+01	2.60E+02
1,2,4-trichlorobenzene	181.45	1.41	3.6	66.4	124.5	4	0.0014	0.03	0.00000823	5.74E+01	4.82E+02
1,2,4-trimethyl benzene	120.20	9.03 ^b	8.97 ^c	35.9 ^c	67.3 ^c	3.63 ^e	0.00616 ^f	0.078 ^c	0.00000903 ^c	2.80E+02	1.30E+04
1,2-bis(ethylthio)-ethene	148.30	0 ^d	6.63 ^c	26.5 ^c	49.7 ^c	2.87 ^f	0.000139 ^k	0.068 ^c	0.00000785 ^c	NA	4.85E+00
1,2-bis(vinylthio)-ethane	146.30	0 ^d	5.92 ^c	23.7 ^c	44.4 ^c	2.82 ^f	0.0000867 ^k	0.068 ^c	0.00000792 ^c	1.99E-10	3.95E+00
1,2-dichlorobenzene	147.00	1.41	3.79	15.2	28.4	3.38	0.0019	0.069	0.0000079	1.81E+02	1.28E+03
1,2-dichlorobutane	127.01	0 ^d	1.77 ^c	7.08 ^c	13.3 ^c	2.74 ^e	0.0214 ^f	0.075 ^c	0.00000871 ^c	2.79E+03	1.51E+04
1,2-dichloroethane	98.96	1.41	0.035	1.52	2.85	1.5	0.00098	0.104	0.0000099	1.05E+04	1.31E+05
1,2-dichloropropane	113.00	0.2	0.09	1.88	3.53	2	0.0028	0.0782	0.00000873	6.93E+03	6.18E+04
1,3-dichlorobenzene	147.00	1.41	8.5	34.0	63.7	3.6	0.0031	0.0692	0.00000786	9.02E+01	4.57E+02
1,4-dichlorobenzene	147.00	1.41	1.2	24.6	46.2	3.5	0.0024	0.069	0.0000079	9.02E+01	5.04E+02
1,4-dioxane	88.11	1.41	0.01	0.02	0.04	-0.27	0.0000048	0.229	0.0000102	5.08E+03	6.52E+07
1,4-dithiane	120.23	0 ^d	0.23 ^c	0.91 ^c	1.71 ^c	1.38 ^e	0.00000491 ^g	0.078 ^c	0.00000903 ^c	2.09E+02	9.81E+04
1,4-oxathiane	104.17	0 ^d	0.03 ^c	0.13 ^c	0.25 ^c	0.53 ^e	0.00000538 ^f	0.086 ^c	0.00000994 ^c	6.15E+02	5.94E+05
1-chlorobutane	92.57	0 ^d	1.48 ^c	5.9 ^c	11.1 ^c	2.64 ^e	0.0167 ^f	0.093 ^c	0.0000108 ^c	1.35E+04	3.61E+04
1-hexene	84.16	0 ^d	5.79 ^c	23.2 ^c	43.4 ^c	3.39 ^e	0.412 ^f	0.099 ^c	0.0000115 ^c	2.45E+04	3.00E+04
2,2-dimethyl-trans-thiirane	88.20	0 ^d	0.45 ^c	1.79 ^c	3.36 ^c	1.68 ^f	0.000611 ^k	0.096 ^c	0.0000111 ^c	NA	1.21E+04
2,3-dimethyl-thiophene	112.20	0 ^d	2.41 ^c	9.66 ^c	18.1 ^c	2.91 ^e	0.00357 ^f	0.082 ^c	0.00000946 ^c	7.88E+02	1.27E+04
2,4,6-trinitrotoluene	227.13	1.41	0.37	1.5	2.8	1.6	0.00000000487	0.001	0.00001	2.70E-04	4.94E+00
2,4-dichlorophenol	163.00	3.61	0.29	5.88	11.0	2.9	0.0000032	0.001	0.00001	1.20E+00	3.48E+01
2,4-dinitrotoluene	182.15	1.41	0.88	3.54	6.63	1.98	0.0000000926	0.203	0.00000706	1.33E-01	2.62E+01
2,6-dinitrotoluene	182.20	1.41	0.49	1.96	3.68	1.72	0.000000747	0.001	0.00001	7.56E-02	4.90E+02
2-butanone	72.11	36.14	0.29	0.08	0.14	0.29	0.000056	0.0808	0.0000098	1.27E+04	3.88E+07
2-chlorobutane	92.57	0 ^d	0.84 ^c	3.35 ^c	6.29 ^c	2.33 ^e	0.0241 ^f	0.093 ^c	0.0000108 ^c	2.09E+04	5.49E+04
2-chloroethoxyethane	187.07	0 ^d	0.18 ^c	0.73 ^c	1.36 ^c	1.28 ^e	0.000000781 ^f	0.058 ^c	0.00000673 ^c	8.00E+00	5.27E+02
2-ethyl 1,3-butadiene	82.14	0 ^d	3.23 ^c	12.9 ^c	24.2 ^c	3.07 ^f	0.245 ^k	0.101 ^c	0.0000116 ^c	1.64E+04	1.01E+04
2-hexanone	100.16	0 ^d	0.23 ^c	0.91 ^c	1.71 ^c	1.38 ^e	0.0000932 ^f	0.088 ^c	0.0000102 ^c	1.55E+03	3.37E+05

Table F-7. Chemical and Physical Properties^a (continued)

COPC	Molecular Weight	Loss Constant due to Degradation	Soil-Water Partition Coefficient	Bed Sediment/ Sediment Pore Water Partition Coefficient	Suspended Sediment-Surface Water Partition Coefficient	Log Octanol-Water Partition Coefficient	Henry's Law Constant	Diffusivity of Chemical in Air	Diffusivity of Chemical in Water	Vapor Pressure	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^h
	(g/mol)	(yr ⁻¹)	(cm ³ water/g soil)	(cm ³ /g/kg)	(l/kg)	(dimensionless)	(atm-m ³ /mol)	(cm ² /s)	(cm ² /s)	(Pa)	(s/cm)
	<i>MW</i>	<i>ksg</i>	<i>Kd_s</i>	<i>Kd_{bs}</i>	<i>Kd_{sw}</i>	<i>log K_{ow}</i>	<i>H</i>	<i>D_a</i>	<i>D_w</i>	<i>V_p</i>	<i>r_{cl}</i>
2-methyl phenol	108.94	36.14	0.83	3.31	6.2	1.95	0.0000012	0.074	0.0000083	4.10E+01	5.58E+01
2-methyl-1,3-dithiacyclopentane	120.20	0 ^d	1.16 ^c	4.64 ^c	8.7 ^c	2.1 ^e	0.00000491 ^e	0.078 ^c	0.00000903 ^c	3.08E+02	2.25E+05
2-methyl-1,3-dithiane	134.30	0 ^d	3.6 ^c	14.4 ^c	26.99 ^c	2.6 ^e	0.00000651 ^e	0.072 ^c	0.00000839 ^c	1.02E+02	6.67E+01
2-methyl-1,3-oxathiolane	104.20	0 ^d	0.03 ^c	0.11 ^c	0.21 ^c	0.46 ^f	0.00000538 ^f	0.086 ^c	0.00000994 ^c	NA	7.15E+04
2-methylnaphthalene	142.20	0 ^d	62.3 ^c	249.3 ^c	467 ^c	3.86 ^e	0.000518 ^e	0.0697 ^c	0.00000807 ^c	7.33E+00	4.71E+02
3-methyl phenol	108.14	8.72	0.85	3.38	6.34	1.96	0.000000865	0.074	0.00001	1.84E+01	3.27E+01
4-methyl phenol	108.14	379.4	12	2.95	5.53	1.9	0.00000079	0.074	0.00001	1.47E+01	2.54E+01
4-methyl-2-pentanone	100.16	36.14	2.2	0.61	1.13	1.2	0.00014	0.075	0.0000078	2.66E+03	8.24E+05
acenaphthylene	152.19	4.94 ^b	74.7 ^c	298.8 ^c	560 ^c	3.94 ^e	0.000114 ^e	0.04386 ^g	0.0000075 ^g	9.00E-01	3.59E+01
acetaldehyde	44.10	0	0.006	0.02	0.05	-0.22	0.0000789	0.124	0.0000141	1.21E+05	1.50E+11
acetone	58.08	36.14	0.087	0.02	0.04	-0.24	0.000039	0.124	0.0000114	3.07E+04	3.36E+08
acetylene	26.04	0 ^d	0.0235 ^c	0.094 ^c	0.176 ^c	0.37 ^e	0.0217 ^e	0.216 ^c	0.0000250 ^c	5.39E+06	1.34E+08
acrolein	56.10	9.03	0.15	0.04	0.07	-0.01	0.00012	0.105	0.0000122	3.60E+04	5.80E+05
alpha-methylstyrene	118.00	0 ^d	6.83 ^c	27.31 ^c	51.2 ^c	3.48 ^e	0.00255 ^e	0.079 ^c	0.00000914 ^c	2.53E+02	7.08E+03
benzene	78.11	15.81	0.12	2.47	4.63	2.1	0.0056	0.088	0.0000102	1.27E+04	2.51E+04
bis(2-chloroisopropyl) ether	171.07	0	3.61 ^c	14.5 ^c	27.1 ^c	2.60	0.000921	0.001	0.00001	1.04E+02	1.07E+05
carbon disulfide	76.10	0	0.091	2.65	4.96	2.2	0.03	0.104	0.00001	4.80E+04	7.45E+02
chlorobenzene	112.56	1.69	0.44	8.96	16.8	2.8	0.0037	0.073	0.0000087	1.58E+03	6.02E+03
chloroethane	64.50	9.03	0.032	0.62	1.15	1.4	0.0088	0.271	0.0000115	1.34E+05	2.11E+04
chloroform	119.38	1.41	0.08	2.1	3.94	2	0.0037	0.104	0.00001	2.66E+04	1.62E+05
chloromethane	50.49	9.03	0.06	0.25	0.47	0.91	0.00882	0.126	0.0000065	5.74E+05	1.89E+06
chloromethoxyethane	94.54	0 ^d	0.06 ^c	0.25 ^c	0.47 ^c	0.81 ^e	0.000403 ^e	0.092 ^c	0.0000106 ^c	7.88E+03	3.17E+05
cis-1,2-dichloroethene	96.94	0	0.071	1.53	2.87	1.9	0.0041	0.001	0.00001	2.67E+04	3.83E+04
dichlorodifluoromethane	120.91	1.41	0.62	2.46	4.61	2.16	0.343	0.001	0.00001	6.47E+05	1.43E+06
diethyl ether	74.12	0 ^d	0.08 ^c	0.3 ^c	0.56 ^c	0.89 ^e	0.000265 ^g	0.0782 ^g	0.0000086 ^g	7.17E+04	5.41E+07
diethyl phthalate	222.24	4.52	44	3.29	6.17	2.5	0.00000045	0.001	0.00001	2.14E-01	4.70E+02
di-n-butyl phthalate	278.35	11	5200	62.8	117.7	4.7	0.0000018	0.0438	0.00000786	9.74E-03	6.46E+01
diphenylamine	169.23	14.45 ^b	27.6 ^c	110.4 ^c	206.9 ^c	3.5 ^e	0.00000269 ^e	0.0621 ^c	0.00000719 ^c	8.93E-02	1.37E+02
ethane	30.07	0 ^d	0.32 ^c	1.3 ^c	2.44 ^c	1.81 ^e	0.5 ^e	0.196 ^c	0.0000228 ^c	4.20E+06	1.65E+03
ethanol	46.07	456.4 ^b	0.00496 ^c	0.0198 ^c	0.0373 ^c	-0.31 ^e	0.000005 ^e	0.123 ^g	0.000013 ^g	7.91E+03	3.29E+09
ethene	28.10	9.03 ^{b,c}	0.09 ^c	0.38 ^c	0.71 ^c	1.13 ^e	0.228 ^e	0.206 ^c	0.0000238 ^e	6.95E+06	2.84E+04
ethyl centralite	268.35	0 ^d	134.5 ^c	538 ^c	1,009 ^c	4.2 ^e	0.000000822 ^g	0.0457 ^c	0.00000529 ^c	2.73E-04	2.75E+01
ethylbenzene	106.20	25.29	0.73	8.16	15.3	3.1	0.0079	0.075	0.0000078	1.28E+03	1.65E+04

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Table F-7. Chemical and Physical Properties^a (continued)

COPC	Molecular Weight	Loss Constant due to Degradation	Soil-Water Partition Coefficient	Bed Sediment/Sediment Pore Water Partition Coefficient	Suspended Sediment-Surface Water Partition Coefficient	Log Octanol-Water Partition Coefficient	Henry's Law Constant	Diffusivity of Chemical in Air	Diffusivity of Chemical in Water	Vapor Pressure	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^h
	(g/mol)	(yr ⁻¹)	(cm ³ water/g soil)	(cm ³ /g/kg)	(l/kg)	(dimensionless)	(atm-m ³ /mol)	(cm ² /s)	(cm ² /s)	(Pa)	(s/cm)
	<i>MW</i>	<i>ksg</i>	<i>K_d_s</i>	<i>K_d_{bs}</i>	<i>K_d_{sw}</i>	<i>log K_{ow}</i>	<i>H</i>	<i>D_a</i>	<i>D_w</i>	<i>V_p</i>	<i>r_{cl}</i>
HD	159.07	23349 ^{b,c}	2.34 ^c	9.36 ^c	17.5 ^c	2.41 ^e	0.000033 ^j	0.065 ^c	0.00000749 ^c	9.33E+00	2.18E+03
hexachlorobutadiene	260.76	1.41	7,600	303.1	568.3	4.8	0.0081	0.0561	0.00000616	2.93E+01	1.45E+04
hexachloroethane	236.74	1.41	15.51	62.0	116.3	3.93	0.00389	0.0025	0.0000068	2.80E+01	2.94E+03
hexane	86.20	0 ^d	14.68 ^c	58.7 ^c	110.1 ^c	3.9 ^e	1.8 ^e	0.097 ^c	0.0000113 ^c	2.01E+04	2.73E+04
methane	16.04	0 ^d	0.087 ^c	0.35 ^c	0.656 ^c	1.09 ^e	0.658 ^e	0.299 ^c	0.0000346 ^c	6.21E+07	8.64E+04
methyl tert-butyl ether	88.20	1.41 ^{b,c}	0.08 ^c	0.34 ^c	0.63e	0.94 ^e	0.000587 ^e	0.096 ^c	0.0000111e	3.33E+04	1.11E+07
methylene chloride	84.93	9.03	0.024	0.4	0.75	1.3	0.0022	0.101	0.0000117	5.74E+04	9.07E+04
monoethanolamine	61.08	0 ^d	0.00051 ^c	0.00206 ^c	0.00387 ^c	-1.31 ^e	0.0000000325 ^e	0.123 ^c	0.0000142 ^c	5.39E+01	6.23E+07
naphthalene	128.17	5.27	300	47.6	89.2	3.3	0.00048	0.059	0.0000075	1.13E+01	3.65E+02
nitrobenzene	123.06	1.28	1.19	4.76	8.93	1.85	0.000024	0.076	0.0000086	2.00E+01	7.51E+02
nitroglycerin	227.09	0 ^d	0.305 ^c	1.22 ^c	2.29 ^c	1.51 ^f	0.00000000254 ^f	0.051 ^c	0.00000591 ^c	5.33E-02	2.90E+00
octane	114.20	0 ^d	151.5 ^c	606.0 ^c	1,136 ^c	5.18 ^e	3.21 ^e	0.081 ^c	0.00000935 ^c	1.88E+03	5.53E+04
pentane	72.20	0 ^d	5.79 ^c	23.2 ^c	43.45 ^c	3.39 ^e	1.25 ^e	0.11 ^c	0.0000127 ^c	6.85E+04	9.67E+03
phenanthrene	178.23	1.26	3700	1061	1,990	4.5	0.000023	0.001	0.00001	1.47E-02	2.33E+01
phenol	94.11	25.29	4.4	1.2	2.24	1.5	0.0000004	0.082	0.0000091	3.73E+01	3.33E+01
propene	42.10	9.03 ^{b,c}	0.3 ^c	1.21 ^c	2.27 ^c	1.77 ^e	0.196 ^e	0.157 ^c	0.0000182 ^c	1.16E+06	1.62E+04
styrene	104.16	9.03	120	36.5	68.4	3	0.0027	0.071	0.000008	8.14E+02	1.13E+04
tert-butyl alcohol	74.10	1.26 ^{b,c}	0.02 ^c	0.09 ^c	0.17 ^c	0.35 ^e	0.00000905 ^e	0.108 ^c	0.0000125 ^c	5.43E+03	2.18E+07
tetracene	228.29	0 ^d	4,596 ^c	18,383 ^c	34,468 ^c	5.76 ^e	0.000000495 ^e	0.0509 ^c	0.00000589 ^c	3.32E-07	3.39E-02
tetrachloroethene	165.83	0.7	0.31	10.6	19.9	3.4	0.018	0.072	0.0000082	2.53E+03	6.04E+03
tetryl	287.15	0 ^d	0.4096 ^c	1.64 ^c	3.07 ^c	1.64 ^e	0.00000000271 ^e	0.0436 ^c	0.00000505 ^c	7.55E-06	1.28E+01
thiirane	60.11	0 ^d	0.06 ^c	0.25 ^c	0.47 ^c	0.81 ^e	0.000346 ^e	0.124 ^c	0.0000143 ^c	3.33E+04	2.84E+06
thiodiglycol	122.18	0 ^d	0.002 ^c	0.01 ^c	0.02 ^c	-0.63 ^e	0.00000000185 ^e	0.077 ^c	0.00000893 ^c	4.31E-01	3.57E+03
toluene	92.14	11.5	0.36	5.6	10.5	2.7	0.0066	0.087	0.0000086	3.73E+03	1.74E+04
trans-1,2-dichloroethene	96.94	0	0.1	1.52	2.85	2.1	0.0094	0.0703	0.0000119	4.40E+04	3.05E+04
trichloroethene	131.39	0.7	0.33	3.77	7.07	2.4	0.01	0.079	0.0000091	9.74E+03	1.88E+04
vinyl chloride	62.50	1.41	0.037	0.62	1.15	1.4	0.027	0.106	0.0000123	4.00E+05	7.35E+03
xylenes	106.16	9.03 ^{b,c}	3.81 ^c	15.2 ^c	28.6	3.16 ^e	0.00663 ^e	0.085 ^c	0.00000981 ^c	1.07E+03	2.00E+04
aluminum	27.00	0 ^d	9.9 ^c	9.9 ^c	9.9 ^c	0.33 ^f	0.0245 ^f	0.211 ^c	0.0000245 ^c	5.65E-07	9.38E+00
ammonia	17.00	0 ^d	0.017 ^c	0.0729 ^c	0.13 ^c	0.23 ^e	0.0000161 ^e	0.287 ^c	0.0000333 ^c	1.00E+06	6.97E+11
arsenic	74.90	0	29	29	29	0.68	0.77	0.0772	0.00000957	3.34E-07	1.57E-02
cadmium	112.40	0	75	75	75	-0.07	0.031	0.0775	0.00000957	5.52E-07	1.62E+10
chlorine	70.91	0	0.25 ^c	0.25 ^c	0.25 ^c	0.85	0.0117	0.001	0.00001	7.77E+05	8.00E+05
copper	63.50	0 ^d	430 ^c	430 ^c	430 ^c	-0.57 ^f	0.0245 ^f	0.119 ^c	0.0000138 ^c	5.65E-07	5.54E+26

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Table F-7. Chemical and Physical Properties^a (continued)

COPC	Molecular Weight	Loss Constant due to Degradation	Soil-Water Partition Coefficient	Bed Sediment/ Sediment Pore Water Partition Coefficient	Suspended Sediment-Surface Water Partition Coefficient	Log Octanol-Water Partition Coefficient	Henry's Law Constant	Diffusivity of Chemical in Air	Diffusivity of Chemical in Water	Vapor Pressure	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^h
	(g/mol)	(yr ⁻¹)	(cm ³ water/g soil)	(cm ³ /g/kg)	(l/kg)	(dimensionless)	(atm-m ³ /mol)	(cm ² /s)	(cm ² /s)	(Pa)	(s/cm)
	<i>MW</i>	<i>ksg</i>	<i>Kd_s</i>	<i>Kd_{bs}</i>	<i>Kd_{sw}</i>	<i>log K_{ow}</i>	<i>H</i>	<i>D_a</i>	<i>D_w</i>	<i>V_p</i>	<i>r_{cl}</i>
hydrogen chloride	36.50	0	0.032 ^c	0.128 ^c	1.22 ^c	0.54 ^f	0.00773 ^f	0.001	0.00001	4.72E+06	3.62E+10
hydrogen cyanide	27.03	0 ^d	0.00568 ^c	0.0227 ^c	0.0426 ^c	-0.25 ^e	0.000133 ^e	0.21 ^c	0.0000244 ^c	9.89E+04	9.01E+12
lead	207.20	0	900	900	900	0.73	0.025	0.0772	0.00000957	4.02E-07	7.07E-01
nickel	58.70	0	65	65	65	-0.57	0.025	0.0772	0.00000957	5.65E-07	1.25E+28
silver	107.90	0	8.3	8.3	8.3	0.23	0.0245 ^f	0.0772	0.00000957	5.65E-07	2.86E+03

- a. USEPA, 2005. *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*, Companion Database. Available online at <http://www.epa.gov/epaoswer/hazwaste/combust/riskvol.htm#volume1>.
- b. Howard et al., 1991. *Handbook of Environmental Degradation Rates*. Lewis Publishers, Chelsea, Michigan.
- c. Calculated using guidance from Appendix A-2 of USEPA, 2005. *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*. Office of Solid Waste and Emergency Response, Washington, DC. EPA530-R-05-006, September 2005.
- d. No data available, *ksg* set to zero as a conservative assumption.
- e. Syracuse Research Corporation, 2003a. PHYSPROP Database. (Available online at <http://www.syrres.com/esc/phsysdemo.htm>).
- f. USEPA, 2000-2007. Estimation Program Interface (EPI) Suite. Copyright © 2000-2007. Available online at <http://www.epa.gov/oppt/exposure/pubs/episuite.html>
- g. USEPA, 1994. *Air Emissions Model for Waste and Wastewater*. Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina. EPA-453/R-94-080A, November 1994.
- h. Derived using the procedure discussed in Section F.4.4.
- i. Syracuse Research Corporation, 2003b. CHEMFATE Database.
- j. Munro et al., 1999, and SAIC, 2006.

Organic Carbon-Water Partition Coefficient. Though not presented in Table F-7, the organic carbon-water partition coefficient is a required calculation because it is used as an intermediate value to derive the soil-water partition coefficient, the bed sediment-sediment pore water partition coefficient, and the suspended sediment-surface water partition coefficient when these values were not directly obtained from the Companion Database to the HHRAP (USEPA, 2005). The organic carbon-water partition coefficient was calculated using the procedures outlined in Appendix A-2 of the HHRAP (USEPA, 2005).

For semi-volatile nonionizing organic compounds, defined as those with a Henry's Law Constant less than 10^{-3} atm-m³/mol, the organic carbon-water partition coefficient was calculated using Equation A-2-7 from the HHRAP (USEPA, 2005), presented below as Equation F-2a:

$$\log K_{oc} = 0.00028 + (0.983 \log K_{ow}) \quad \text{Eq. F-2a}$$

where

$$\begin{aligned} K_{oc} &= \text{organic carbon-water partition coefficient (cm}^3\text{/g)} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

For volatile nonionizing organic compounds, defined as those with a Henry's Law Constant greater than 10^{-3} atm-m³/mol, chlorinated benzenes, and certain pesticides, the organic carbon-water partition coefficient was calculated using Equation A-2-8 from the HHRAP (USEPA, 2005), presented below as Equation F-2b:

$$\log K_{oc} = 0.0784 + (0.7919 \log K_{ow}) \quad \text{Eq. F-2b}$$

where

$$\begin{aligned} K_{oc} &= \text{organic carbon-water partition coefficient (cm}^3\text{/g)} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

Soil-Water Partition Coefficient. When available, the soil-water partition coefficient was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). When no value was available in the Companion Database, the soil-water partition coefficient was calculated using Equation A-2-10 from the HHRAP (USEPA, 2005), presented below as Equation F-3:

$$Kd_s = f_{oc,s} \cdot K_{oc} \quad \text{Eq. F-3}$$

where

$$\begin{aligned} Kd_s &= \text{soil-water partition coefficient (cm}^3\text{/g)} \\ f_{oc,s} &= \text{fraction of organic carbon in soils} \\ K_{oc} &= \text{organic carbon-water partition coefficient (cm}^3\text{/g)} \end{aligned}$$

Section A2-2.10, Appendix A-2 of the of the HHRAP (USEPA, 2005), states that based on previous literature searches, the fraction of organic carbon in soil ranges from 0.002 to 0.024; from this range, a mid-range value of 0.01 generally can be used. This mid-range value was used when the soil-water partition coefficient was calculated using this procedure.

Bed Sediment-Sediment Pore Water Partition Coefficient. When available, the bed sediment-sediment pore water partition coefficient was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). When data were unavailable in the Companion Database, the bed sediment-sediment pore water partition coefficient was calculated using Equation A-2-12 from the HHRAP (USEPA, 2005), presented below as Equation F-4:

$$Kd_{bs} = f_{oc,bs} \cdot K_{oc} \quad \text{Eq. F-4}$$

where

Kd_{bs}	=	bed sediment-sediment pore water partition coefficient (cm ³ /g/kg)
$f_{oc, bs}$	=	fraction of organic carbon in bottoms sediment
K_{oc}	=	organic carbon-water partition coefficient (cm ³ /g)

Section A2-2.10, Appendix A-2 of the HHRAP (USEPA, 2005), states that based on previous literature searches, the fraction of organic carbon in bottoms sediment ranges from 0.03 to 0.05; from this range, a mid-range value of 0.04 generally can be used. This mid-range value was used when the bed sediment-sediment pore water partition coefficient was calculated using this procedure.

Suspended Sediment-Surface Water Partition Coefficient. When available, the suspended sediment-surface water partition coefficient was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). When a value was not available in the Companion Database, the suspended sediment-surface water partition coefficient was calculated using Equation A-2-11 from the HHRAP (USEPA, 2005), presented below as Equation F-5:

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \quad \text{Eq. F-5}$$

where

Kd_{sw}	=	suspended sediment-surface water partition coefficient (l/kg)
$f_{oc, sw}$	=	fraction of organic carbon in suspended sediments
K_{oc}	=	organic carbon-water partition coefficient (cm ³ /g)

Section A2-2.10, Appendix A-2 of the HHRAP (USEPA, 2005), states that based on previous literature searches, the fraction of organic carbon in suspended sediments ranges from 0.05 to 0.1; from this range, a mid-range value of 0.075 generally can be used. This mid-range value was used when the suspended sediment-surface water partition coefficient was calculated using this procedure.

Diffusivity of Chemical in Air. When available, the diffusivity of a chemical in air was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005) or from the *Air Emission Model for Waste and Wastewater* (USEPA, 1994). In the absence of values from either of these sources, the diffusivity of the chemical in air was estimated using Equation A-2-4 from the HHRAP (USEPA, 2005), presented as Equation F-6 below:

$$D_a = \frac{1.9}{(MW)^{2/3}} \quad \text{Eq. F-6}$$

where

$$\begin{aligned} D_a &= \text{diffusivity of chemical in air (cm}^2\text{/second)} \\ MW &= \text{molecular weight of chemical (g/mol)} \end{aligned}$$

Diffusivity of Chemical in Water. When available, the diffusivity of a chemical in water was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005) or from the *Air Emission Model for Waste and Wastewater*. In the absence of values from either of these sources, the diffusivity of the chemical in water was calculated using Equation A-2-5 from the HHRAP (USEPA, 2005), presented as Equation F-7 below:

$$D_w = \frac{22 \cdot 10^{-5}}{(MW)^{2/3}} \quad \text{Eq. F-7}$$

where

$$\begin{aligned} D_w &= \text{diffusivity of chemical in water (cm}^2\text{/second)} \\ MW &= \text{molecular weight of chemical (g/mol)} \end{aligned}$$

Fraction of Air Concentration that is in the Vapor Phase. When available, the fraction of COPC air concentration in the vapor phase (F_v) was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). For those COPCs not included in the Companion Database, F_v was calculated using the procedures provided in Appendix A-2 of the HHRAP. For most COPCs, which are a liquid at ambient temperature, F_v was calculated using Equation A-2-1 from the HHRAP (USEPA, 2005), presented as Equation F-8 below:

$$F_v = 1 - \frac{cS_T}{V_p + cS_T} \quad \text{Eq. F-8}$$

where

$$\begin{aligned} F_v &= \text{fraction of air concentration in the vapor phase (dimensionless)} \\ c &= \text{Junge constant (1.7x10}^{-4}\text{ atm-cm)} \\ S_T &= \text{Whitby's average surface area of particulates (cm}^2\text{/cm}^3\text{)} \\ V_p &= \text{vapor pressure (atm)} \end{aligned}$$

Whitby's average surface area of particulates can vary by several orders of magnitude from 10^{-4} to 10^{-8} depending on the particle concentration in an area. For calculations in the MPHRA, a value of 10^{-6} was used to be representative of a rural site (Junge, 1977).

Equation F-8 resulted in a value of 1.0 for F_v for all COPCs except for the metal COPCs.

For all metal COPCs, which are present predominately in the particulate phase and not in the vapor phase, F_v was assumed to be zero, as recommended in *Appendix A-2 of the HHRAP*.

Table F-8. Biotransfer Factors^a

COPC	Air-to-Plant Biotransfer Factor	Plant-Soil Bio-Concentration Factor for Above-Ground Produce	Root Concentration Factor	Biotransfer Factor for Beef	Biotransfer Factor for Milk	Biotransfer Factor for Eggs	Biotransfer Factor for Pork	Biotransfer Factor for Chicken	Bio-Concentration Factor
	(mg/kg)/(ug/g)	(mg/kg)/(ug/g)	(dimensionless)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(ℓ/kg)
	<i>B_{vag}</i>	<i>B_r</i>	<i>RCF</i>	<i>B_a^{beef}</i>	<i>B_a^{milk}</i>	<i>B_a^{egg}</i>	<i>B_a^{pork}</i>	<i>B_a^{chicken}</i>	<i>BCF_{fish}</i>
1,1,1,2-tetrachloroethane	0.039	0.687	50	1.13	2.37	4.75	1.36	8.30	43
1,1,1-trichloroethane	0.00151	1.39	19.5	5.96	1.25	2.50807	0.0072107	4.3891	16.8
1,1,2,2-tetrachloroethane	0.0591	1.59	16.4	0.00521	0.0011	0.00219	0.0063	0.00384	14.1
1,1-dichloroethane	0.000825	3.53	12	0.00211	0.000444	0.000888	0.00255	0.00155	4.85
1,1-dichloroethene	0.000371	2.37	9.62	3.38	0.000712	1.424	4.0939	2.4919	8.26
1,2,3-trichlorobenzene	0.92	0.177	305	0.0268	0.00564	0.0113	0.0325	0.0198	262
1,2,4-trichlorobenzene	0.727	0.189	279	0.026	0.00547	0.0109	0.0314	0.0191	240
1,2,4-trimethyl benzene	0.0666	0.31	144.93	0.0199	0.00418	0.00837	0.0241	0.0146	124.5
1,2-bis(ethylthio)-ethene ^b	0.458	0.85	37.67	0.00942	0.00198	0.00397	0.0114	0.00694	32.4
1,2-bis(vinylthio)-ethane ^b	0.649	0.91	34.47	0.00889	0.00187	0.00374	0.0108	0.00655	29.6
1,2-dichlorobenzene	0.117	0.431	93	0.0160	0.00337	0.00674	0.0194	0.0118	79.9
1,2-dichlorobutane ^b	0.00216	1.01	29.9	0.00808	0.0017	0.0034	0.00978	0.00595	25.7
1,2-dichloroethane	0.00226	5.26	9.63	0.00126	0.000266	0.000531	0.00153	0.00093	2.85
1,2-dichloropropane	0.00269	2.7	8.05	0.0029	0.000611	0.00122	0.00351	0.00214	6.92
1,3-dichlorobenzene	0.123	0.322	137	0.0194	0.00408	0.00817	0.0235	0.0143	118
1,4-dichlorobenzene	0.124	0.367	115	0.0178	0.01782	0.00750	0.02163	0.0131	98.9
1,4-dioxane	0.00601	8.38	6.45	0.0000265	0.00000557	0.0000111	0.000032	0.0000195	3.16
1,4-dithiane ^b	0.336	6.17	8.99	0.00102	0.000214	0.000428	0.00123	0.000749	2.3
1,4-oxathiane ^b	0.0381	19.1	6.9	0.000181	0.0000381	0.0000763	0.000219	0.000133	3.16
1-chlorobutane ^b	0.00217	1.15	25.05	0.00714	0.0015	0.00301	0.00864	0.00526	21.5
1-hexene ^b	0.000553	0.43	94.7	0.0162	0.0034	0.0068	0.0196	0.0119	81.3
2,2-dimethyl-trans-thiirane ^b	0.00563	4.14	10.9	0.00173	0.000363	0.000727	0.00209	0.00127	3.92
2,3-dimethyl-thiophene ^b	0.0197	0.81	40.4	0.00987	0.00208	0.00415	0.0119	0.00727	34.7
2,4,6-trinitrotoluene	581	4.6	10.3	1.50	0.000317	0.000633	1.82	1.11	3.4
2,4-dichlorophenol	21.4	0.816	39.7	0.00571	0.00120	0.00241	0.00692	0.00421	13.6
2,4-dinitrotoluene	77.5	2.78	14.1	2.8134	0.000592	1.185	3.40	2.07	6.68
2,6-dinitrotoluene	5.08	3.93	11.2	1.8462	0.000389	0.000777	2.2348	1.36034	4.21
2-butanone	0.00203	8.38	6.7	0.000105	0.0000221	0.0000442	0.000127	0.0000773	3.16
2-chlorobutane ^b	0.000703	1.74	14.5	0.00472	0.000995	0.00199	0.00572	0.00348	12.4
2-chloroethoxyethane ^b	1.65	7.05	8.55	0.000844	0.000178	0.000355	0.00102	0.000622	1.93
2-ethyl 1,3-butadiene ^b	0.000425	0.65	53.7	0.0118	0.00248	0.00495	0.0142	0.00867	46.1
2-hexanone ^b	0.0177	6.17	8.99	0.00102	0.000214	0.000428	0.00123	0.000749	2.3

Table F-8. Biotransfer Factors^a (continued)

COPC	Air-to-Plant Biotransfer Factor	Plant-Soil Bio-Concentration Factor for Above-Ground Produce	Root Concentration Factor	Biotransfer Factor for Beef	Biotransfer Factor for Milk	Biotransfer Factor for Eggs	Biotransfer Factor for Pork	Biotransfer Factor for Chicken	Bio-Concentration Factor
	(mg/kg)/(ug/g)	(mg/kg)/(ug/g)	(dimensionless)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(l/kg)
	<i>B_{vag}</i>	<i>B_r</i>	<i>RCF</i>	<i>B_a^{beef}</i>	<i>B_a^{milk}</i>	<i>B_a^{egg}</i>	<i>B_a^{pork}</i>	<i>B_a^{chicken}</i>	<i>BCF_{fish}</i>
2-methyl phenol	5.56	2.89	13.7	2.68	0.000564	1.1284	3.2441	1.9747	6.33
2-methyl-1,3-dithiacyclopentane ^b	1.96	2.37	9.62	0.00338	0.000712	0.00142	0.00409	0.00249	8.26
2-methyl-1,3-dithiane ^b	5.04	1.22	23.3	0.00678	0.00143	0.00286	0.00821	0.005	20.0
2-methyl-1,3-oxathiolane ^b	0.0312	21	6.83	0.000155	0.0000326	0.0000652	0.000187	0.000114	3.16
2-methylnaphthalene ^b	1.39	0.227	217	0.0237	0.00498	0.00996	0.0286	0.0174	187
3-methyl phenol	7.9	2.85	13.8	0.00273	0.000574	0.00115	0.0033	0.00201	6.44
4-methyl phenol	7.47	3.09	13.05	0.00248	0.000522	0.00104	0.003	0.00183	5.79
4-methyl-2-pentanone	0.00757	7.84	8.26	0.000725	0.000153	0.000305	0.000877	0.000534	1.67
acenaphthylene ^b	7.70	0.204	251	0.0250	0.00526	0.0105	0.03026	0.0184	216
acetaldehyde	0.000413	8.38	6.46	0.0000301	0.00000634	0.0000127	0.0000364	0.0000222	3.16
acetone	0.000796	8.38	6.46	0.0000286	0.00000602	0.000012	0.0000346	0.0000211	3.16
acetylene ^b	0.00105	8.38	0.878	0.000126	0.0000266	0.0000531	0.000153	0.0000930	3.16
acrolein	0.000455	8.38	6.54	0.0000511	0.0000107	0.0000215	0.0000618	0.0000376	3.16
alpha-methylstyrene ^b	0.111	0.38	111	0.0175	0.00369	0.00737	0.0212	0.0129	95.4
benzene	0.00172	2.37	9.62	0.00338	0.000712	0.00142	0.00409	0.00249	8.26
bis(2-chloroisopropyl) ether	0.0358	1.21	23.4	0.00680	0.00143	0.00286	0.00823	0.00501	20.1
carbon disulfide	0.00041	2.07	11.5	0.00392	0.000826	0.00165	0.00475	0.00289	9.86
chlorobenzene	0.0145	0.932	33.3	8.6815	1.83	3.65	1.05	6.40	28.6
chloroethane	0.000197	6.01	9.09	0.00105	0.000222	0.000444	0.00128	0.000776	2.39
chloroform	0.00204	2.7	8.05	0.0029	0.000611	0.00122	0.00351	0.00214	6.92
chloromethane	0.000059	8.38	7.47	0.000408	0.0000858	0.000172	0.000494	0.0003	3.16
chloromethoxyethane ^b	0.00101	13.18	7.28	0.000332	0.0000698	0.00014	0.000401	0.000244	3.16
cis-1,2-dichloroethene	0.00144	3.09	13.1	0.00248	0.000522	0.00104	0.00300	0.00183	5.79
dichlorodifluoromethane	0.0000325	2.19	10.7	0.00370	0.000779	1.56	4.48	2.72	9.19
diethyl ether ^b	0.0187	11.85	7.43	0.000391	0.0000824	0.000165	0.000474	0.000288	3.16
diethyl phthalate	57.1	1.39	19.5	5.96	1.25	2.51	0.00721	4.39	16.8
di-n-butyl phthalate	3150	0.074	966	3.64	7.66	1.53	4.40	0.0268	830
diphenylamine ^b	111.0	0.367	115	0.0178	0.00375	0.00750	0.0216	0.0131	98.8
ethane ^b	0.00000946	3.48	12.1	0.00214	0.000451	0.000903	0.00259	0.00158	4.94
ethanol ^b	0.00523	58.5	6.44	0.0000238	0.00000502	0.0000100	0.0000289	0.0000176	3.16
ethene ^b	0.00000392	8.61	8.03	0.000633	0.000133	0.000267	0.000766	0.000466	1.48
ethyl centralite ^b	20212	0.145	398	0.0293	0.00616	0.0123	0.0354	0.0216	342
ethylbenzene	0.0142	0.625	56.6	0.0121	0.00256	0.00511	0.0147	0.00895	48.6

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Table F-8. Biotransfer Factors^a (continued)

COPC	Air-to-Plant Biotransfer Factor	Plant-Soil Bio-Concentration Factor for Above-Ground Produce	Root Concentration Factor	Biotransfer Factor for Beef	Biotransfer Factor for Milk	Biotransfer Factor for Eggs	Biotransfer Factor for Pork	Biotransfer Factor for Chicken	Bio-Concentration Factor
	(mg/kg)/(ug/g)	(mg/kg)/(ug/g)	(dimensionless)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(l/kg)
	<i>B_{vag}</i>	<i>B_r</i>	<i>RCF</i>	<i>B_a^{beef}</i>	<i>B_a^{milk}</i>	<i>B_a^{egg}</i>	<i>B_a^{pork}</i>	<i>B_a^{chicken}</i>	<i>BCF_{fish}</i>
HD ^b	0.624	1.57	16.7	0.00528	0.00111	0.00222	0.00639	0.00389	14.3
hexachlorobutadiene	0.893	0.065	1150	0.0375	0.00789	0.0158	0.0454	0.0276	991
hexachloroethane	0.22	0.207	247	0.0248	0.00522	0.0104	0.03	0.0183	212
hexane ^b	0.000442	0.22	243	0.0243	0.00512	0.0102	0.0294	0.0179	200.9
methane ^b	0.0000123	9.08	7.91	0.000585	0.0000445	0.0000089	0.0000256	0.0000156	1.38
methyl tert-butyl ether ^b	0.000954	11.08	7.54	0.000434	0.0000913	0.000183	0.000525	0.000319	3.16
methylene chloride	0.000616	6.86	8.64	0.000876	0.000184	0.000369	0.00106	0.000645	2
monoethanolamine ^b	1.18	8.38	0.831	0.00000906	0.00000191	0.00000382	0.0000110	0.00000668	3.16
naphthalene	0.381	0.479	80.7	0.0148	0.00312	0.00625	0.018	0.0109	69.3
nitrobenzene	0.217	3.3	12.5	0.00229	0.00229	0.000963	0.00277	0.00168	5.3
nitroglycerin ^b	893	5.19	9.69	0.00128	0.000270	0.000541	0.00155	0.000946	2.90
octane ^b	0.00572	0.04	2263	0.0403	0.00848	0.017	0.0487	0.0297	1,943
pentane ^b	0.000182	0.43	94.7	0.0162	0.0034	0.0068	0.0196	0.0119	81.3
phenanthrene	151	0.097	678	0.0338	0.00712	0.0142	0.0409	0.0249	582
phenol	5.53	5.26	9.63	0.00126	0.000265	0.000530	0.00152	0.000928	2.85
propene ^b	0.0000219	3.67	11.7	0.00201	0.000422	0.000845	0.00243	0.00148	4.6
styrene	0.0324	0.714	47.4	1.09	2.30	4.59	1.32	8.0376	40.7
tert-butyl alcohol ^b	0.0146	24.3	6.74	0.000121	0.0000254	0.0000508	0.000146	0.0000888	3.16
tetracene ^b	153912	0.0181	6328	0.0396	0.00833	0.01667	0.0479	0.0291	5,435
tetrachloroethene	0.013	0.42	96.4	0.0163	0.00343	0.00686	0.0197	0.012	82.8
tetryl ^b	1151	4.36	10.6	0.00161	0.000339	0.000679	0.00195	0.00119	3.65
thiirane ^b	0.00118	13.2	7.28	0.000332	0.0000698	0.00014	0.000401	0.000244	3.16
thiodiglycol ^b	6.44	89.6	6.38	0.0000101	0.00000213	0.00000426	0.0000123	0.00000746	3.16
toluene	0.00636	1.07	27.9	0.00769	0.00162	0.00324	0.00931	0.00567	23.9
trans-1,2-dichloroethene	0.00103	2.37	9.62	0.00338	0.000712	0.00142	0.00409	0.00249	8.26
trichloroethene	0.00201	1.59	16.4	0.00521	0.0011	0.00219	0.0063	0.00384	14.1
vinyl chloride	0.0000641	6.01	9.09	0.00105	0.000222	0.000444	0.00128	0.000776	2.39
xylenes ^b	0.0195	0.578	63.0	0.0129	0.00272	0.00544	0.0156	0.00952	54.1
aluminum ^b	NA	0.00108	0.00643	0.0015	0.0002	0	0	0	3.16
ammonia ^b	NA	28.5	6.66	0	0	0	0	0	3.16
arsenic	NA	0.00633	0.174	0.002	0.00006	0	0	0	114
cadmium	NA	0.125	11.2	0.00012	0.0000065	0.0025	0.000191	0.106	907
chlorine	NA	8.38	7.36	0.00036	0.0000759	0.000152	0.000436	0.000266	3.16
copper ^b	NA	0.269	107	0.01	0.0015	0	0	0	3.16

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Table F-8. Biotransfer Factors^a (continued)

COPC	Air-to-Plant Biotransfer Factor	Plant-Soil Bio-Concentration Factor for Above-Ground Produce	Root Concentration Factor	Biotransfer Factor for Beef	Biotransfer Factor for Milk	Biotransfer Factor for Eggs	Biotransfer Factor for Pork	Biotransfer Factor for Chicken	Bio-Concentration Factor
	(mg/kg)/(ug/g)	(mg/kg)/(ug/g)	(dimensionless)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(day/kg)	(l/kg)
	<i>B_{vag}</i>	<i>B_r_{ag}</i>	<i>RCF</i>	<i>B_a_{beef}</i>	<i>B_a_{milk}</i>	<i>B_a_{egg}</i>	<i>B_a_{pork}</i>	<i>B_a_{chicken}</i>	<i>BCF_{fish}</i>
hydrogen chloride ^b	NA	18.9	6.91	0.0000523	0.000011	0.000022	0.0000633	0.0000386	3.16
hydrogen cyanide ^b	8.2281	147.7	0.839	0	0	0	0	0	3.16
lead	NA	0.0136	8.1	0.0003	0.00025	0	0	0	0.09
nickel	NA	0.00931	3.9	0.006	0.001	0	0	0	78
silver	NA	0.138	0.83	0.003	0.02	0	0	0	87.7

a. USEPA, 2005. *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*, Companion Database. Available online at <http://www.epa.gov/epaoswer/hazwaste/combust/riskvol.htm#volume1>.

b. Based on guidance from Appendix A-2 of USEPA, 2005. *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*. Office of Solid Waste and Emergency Response, Washington, DC. EPA530-R-05-006, September 2005.

F.4.2 Transfer Factors

Table F-8 presents transfer factors for all COPCs identified in the MPHRA obtained from various sources and used to evaluate the overall excess lifetime cancer risk and HI for each exposure scenario. Generally, transfer factors were obtained from the Companion Database to the HHRAP (USEPA, 2005). When transfer factors were not available in the Companion Database, parameters were calculated using the procedures described in Appendix A-2 of the HHRAP (USEPA, 2005). The following sections discuss the procedures used when parameters in Table F-8 were calculated.

Volumetric Air-to-Plant Biotransfer Factor. Though not presented in Table F-8, the volumetric air-to-plant biotransfer factor is a required calculation because it is used as an intermediate value to calculate the air-to plant biotransfer factor when this value was not directly obtained from the Companion Database to the HHRAP (USEPA, 2005). The volumetric air-to-plant biotransfer factor was calculated using Equation A-2-19 from the HHRAP (USEPA, 2005) at a temperature of 25°C, and presented as Equation F-9 below:

$$\log B_{vol} = 1.065 \log K_{ow} - \log \left(\frac{H}{RT} \right) - 1.654 \quad \text{Eq. F-9}$$

where

B_{vol}	=	volumetric air-to-plant biotransfer factor (fresh weight basis)
$\log K_{ow}$	=	log of the octanol-water partition coefficient (dimensionless)
H	=	Henry's Law Constant (atm-m ² /mol)
R	=	universal gas constant (atm-m ² /mol-K)
T	=	temperature (K)

Air-to-Plant Biotransfer Factor. When available, the air-to-plant biotransfer factor was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the air-to-plant biotransfer factor was calculated using Equation A-2-20 from the HHRAP (USEPA, 2005), presented as Equation F-10 below:

$$Bv_{ag} = \frac{\rho_{air} B_{vol}}{100(1 - f_{water})\rho_{forage}} \quad \text{Eq. F-10}$$

where

Bv_{ag}	=	air-to-plant biotransfer factor ([mg COPC/kg dry weight plant]/[µg COPC/g air])
ρ_{air}	=	density of air (1.19 g/ℓ)
B_{vol}	=	volumetric air-to-plant biotransfer factor (fresh weight basis)
f_{water}	=	fraction of forage that is water (0.85 dimensionless)
ρ_{forage}	=	density of forage (770 g/ℓ)

Equation A-2-20 is not reduced by a factor of 100 in Appendix A-2 of the HHRAP (USEPA, 2005). A reduction factor of 100 is applied to Equation F-10 because Section A2-2.12.4, Appendix A-2 of the HHRAP (USEPA, 2005), recommends reducing the air-to-plant biotransfer factor calculated by Equation A-2-20 by a factor of 100.

Plant-Soil Bioconcentration Factor for Aboveground Produce. When available, the plant-soil bioconcentration factor for above-ground produce was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the plant-soil bioconcentration factor for above-ground produce was calculated using Equation A-2-17 from the HHRAP (USEPA, 2005), presented as Equation F-11 below:

$$\log Br_{ag} = 1.588 - 0.578 \log K_{ow} \quad \text{Eq. F-11}$$

where

$$\begin{aligned} Br_{ag} &= \text{plant-soil bioconcentration factor for above-ground produce} \\ &\quad \text{(mg/kg / } \mu\text{g/g)} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

Root Concentration Factor. When available, the root concentration factor was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the root concentration factor was calculated using Equation A-2-14 or Equation A-2-15 from the HHRAP (USEPA, 2005), presented as Equation F-12a and Equation F-12b below.

In agreement with Appendix A-2 of the HHRAP (USEPA, 2005), for compounds with $\log K_{ow}$ values greater than 2.0, the root concentration factor was calculated using Equation F-12a.

$$\log (0.13RCF) = 0.77 \log K_{ow} - 1.52 \quad \text{Eq. F-12a}$$

where

$$\begin{aligned} RCF &= \text{root concentration factor (dimensionless, dry weight basis)} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

For compounds with $\log K_{ow}$ values less than 2.0, the root concentration factor was calculated using Equation F-12b, presented below:

$$\log (0.13RCF - 0.82) = 0.77 \log K_{ow} - 1.52 \quad \text{Eq. F-12b}$$

where

$$\begin{aligned} RCF &= \text{root concentration factor (dimensionless, dry weight basis)} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

Equations A-2-14 and A-2-15, as presented in Appendix A-2 of the HHRAP (USEPA, 2005), are used to calculate the root concentration factor on a fresh-weight basis, but subsequent calculations use the root concentration factor on a dry-weight basis. Section A2-2.12.1 of Appendix A of the HHRAP (USEPA, 2005) recommends that the calculated root concentration factor be converted to a dry-weight basis using a moisture concentration of 87 percent in root vegetables. Equations F-12a and Equation F-12b have been modified to include the multiplier of 0.13 to accomplish this conversion.

Log of the Biotransfer Factor for Fat. Though not presented in Table F-8, the log of the biotransfer factor for fat is a required calculation because it is used as an intermediate value to calculate the biotransfer factors for beef, milk, pork, chicken, and eggs when these values were not directly obtained from the Companion Database to the HHRAP (USEPA, 2005). The biotransfer factor for fat was calculated using Equation A-2-21 from the HHRAP (USEPA, 2005), presented below as Equation F-13.

$$\log Ba_{fat} = -0.099(\log K_{ow})^2 + 1.07 \log K_{ow} - 3.56 \quad \text{Eq. F-13}$$

where

$$\begin{aligned} Ba_{fat} &= \text{biotransfer factor for fat ((mg/kg fat)/(mg/day))} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

Biotransfer Factor for Beef. When available, the biotransfer factor for beef was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the biotransfer factor for beef was calculated using Equation A-2-23 from the HHRAP (USEPA, 2005), presented as Equation F-14 below:

$$Ba_{beef} = 0.19 \cdot 10^{\log Ba_{fat}} \quad \text{Eq. F-14}$$

where

$$\begin{aligned} Ba_{beef} &= \text{biotransfer factor for beef (day/kg)} \\ Ba_{fat} &= \text{biotransfer factor for fat ((mg/kg fat)/(mg/day))} \end{aligned}$$

Biotransfer Factor for Milk. When available, the biotransfer factor for milk was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the biotransfer factor for milk was calculated using Equation A-2-22 from the HHRAP (USEPA, 2005), presented as Equation F-15 below:

$$Ba_{milk} = 0.04 \cdot 10^{\log Ba_{fat}} \quad \text{Eq. F-15}$$

where

$$\begin{aligned} Ba_{milk} &= \text{biotransfer factor for dairy milk (day/kg)} \\ Ba_{fat} &= \text{biotransfer factor for fat ((mg/kg fat)/(mg/day))} \end{aligned}$$

Biotransfer Factor for Eggs. When available, the biotransfer factor for eggs was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the biotransfer factor for eggs was calculated using Equation A-2-28 from the HHRAP (USEPA, 2005), presented as Equation F-16 below:

$$Ba_{egg} = 0.08 \cdot 10^{\log Ba_{fat}} \quad \text{Eq. F-16}$$

where

$$\begin{aligned} Ba_{egg} &= \text{biotransfer factor for eggs (day/kg)} \\ Ba_{fat} &= \text{biotransfer factor for fat ((mg/kg fat)/(mg/day))} \end{aligned}$$

Biotransfer Factor for Pork. When available, the biotransfer factor for pork was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the biotransfer factor for pork was calculated using Equation A-2-26 from the HHRAP (USEPA, 2005), presented as Equation F-17 below:

$$Ba_{pork} = 0.23 \cdot 10^{\log Ba_{fat}} \quad \text{Eq. F-17}$$

where

$$\begin{aligned} Ba_{pork} &= \text{biotransfer factor for pork (day/kg)} \\ Ba_{fat} &= \text{biotransfer factor for fat ((mg/kg fat)/(mg/day))} \end{aligned}$$

Biotransfer Factor for Chicken. When available, the biotransfer factor for chicken was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the biotransfer factor for chicken was calculated using Equation A-2-26 from the HHRAP (USEPA, 2005), presented as Equation F-18 below:

$$Ba_{chick} = 0.14 \cdot 10^{\log Ba_{fat}} \quad \text{Eq. F-18}$$

where

$$\begin{aligned} Ba_{chick} &= \text{biotransfer factor for chicken (day/kg)} \\ Ba_{fat} &= \text{biotransfer factor for fat ((mg/kg fat)/(mg/day))} \end{aligned}$$

Bioconcentration Factors for Fish. When available, the bioconcentration factor for fish was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the bioconcentration factor for fish was calculated using Equation A-2-27 or Equation A-2-28 from the HHRAP (USEPA, 2005), presented as Equation F-19a and Equation F-19b below.

As described by Appendix A-2 of the HHRAP (USEPA, 2005), for compounds with $\log K_{ow}$ values less than 1.0, the bioconcentration factor for fish was calculated using Equation F-19a.

$$\log BCF_{fish} = 0.50 \quad \text{Eq. F-19a}$$

where

$$BCF_{fish} = \text{bioconcentration factor for fish (l/kg)}$$

For compounds with $\log K_{ow}$ values greater than or equal to 1.0, but less than 7.0, the bioconcentration factor for fish was calculated by Equation F-19b, presented below:

$$\log BCF_{fish} = 0.77 \log K_{ow} - 0.70 \quad \text{Eq. F-19b}$$

where

$$BCF_{fish} = \text{bioconcentration factor for fish (l/kg)}$$

Fraction of COPC that is Freely Dissolved in Water. Though not presented in Table F-8, the fraction of a COPC that is freely dissolved in water is a required calculation because it is used

as an intermediate value to calculate the bioaccumulation factor when this value was not directly obtained from the Companion Database to the HHRAP (USEPA, 2005). The fraction of a COPC that is freely dissolved in water was calculated using Equation A-2-36 from the HHRAP (USEPA, 2005), presented below as Equation F-20:

$$f_{fd} = \frac{1}{1 + \frac{(DOC)(K_{ow})}{10} + (POC)(K_{ow})} \quad \text{Eq. F-20}$$

where

f_{fd}	=	fraction of chemical that is freely dissolved in water (dimensionless)
DOC	=	dissolved organic carbon (kg organic carbon/ℓ)
K_{ow}	=	octanol-water partition coefficient (dimensionless)
POC	=	particulate organic carbon (kg organic carbon/ℓ)

Section A2-2.13.4.2 of Appendix A-2 of the HHRAP (USEPA, 2005) recommends values for the concentration of dissolved organic carbon and the concentration of particulate organic carbon of 2×10^{-6} kilograms per liter (kg/ℓ) and 7.5×10^{-9} kg/ℓ, respectively.

Bioaccumulation Factor for Fish. When available, the bioaccumulation factor for fish was obtained for each COPC from the Companion Database to the HHRAP (USEPA, 2005). In the absence of values from this source, the bioaccumulation factor was calculated using Equation A-2-37 from the HHRAP (USEPA, 2005), presented as Equation F-21 below:

$$BAF_{fish} = \frac{BCF_{fish} - 1}{f_{fd}} \quad \text{Eq. F-21}$$

where

BAF_{fish}	=	bioaccumulation factor for fish (ℓ/kg)
BCF_{fish}	=	bioconcentration factor for fish(ℓ/kg)

Equation A-2-37 in the HHRAP (USEPA, 2005) presents $BAF(dissolved)$ and $BAF(total)$ instead of BAF and BCF as presented in Equation F-21. For this MPHRA, the assumption has been made that $BAF(dissolved)$ is equal to BCF . Only seven COPCs require a bioaccumulation factor:

▪ 1,2,3-trichlorobenzene:	$BAF_{fish} = 344.69 \text{ ℓ/kg}$
▪ di-n-butyl phthalate:	$BAF_{fish} = 1,800 \text{ ℓ/kg}$
▪ ethyl centralite:	$BAF_{fish} = 342.10 \text{ ℓ/kg}$
▪ hexachlorobutadiene:	$BAF_{fish} = 2,430 \text{ ℓ/kg}$
▪ octane:	$BAF_{fish} = 2,003.61 \text{ ℓ/kg}$
▪ phenanthrene:	$BAF_{fish} = 1,027.99 \text{ ℓ/kg}$
▪ tetracene:	$BAF_{fish} = 6,082.97 \text{ ℓ/kg}$

Biota-to-Sediment Accumulation Factor. The biota-to-sediment accumulation factor was not obtained for any COPCs because the HHRAP (USEPA, 2005) recommends the use of a biota-to-sediment accumulation factor only when the COPC is a dioxin, furan, or polychlorinated biphenyl (PCB). None of the COPCs evaluated in this MPHRA are dioxins, furans, or PCBs.

Empirical Correction Factor for Above-ground Produce. Though not presented in Table F-8, the empirical correction factor for above-ground produce, VG_{ag} , is a chemical-specific value used in calculations in the MPHRA. The HHRAP (USEPA, 2005) recommends that for COPCs with $\log K_{ow}$ greater than 4.0, the empirical correction factor should be assigned a value of 0.01 (dimensionless), and for COPCs with $\log K_{ow}$ less than 4.0, the empirical correction factor should be assigned a value of 1.0. The following COPCs have $\log K_{ow}$ greater than 4.0 and were assigned a value of 0.01 (dimensionless) in the MPHRA for the empirical correction factor for above-ground produce:

- 1,2,3-trichlorobenzene
- HD
- octane

All of the remaining COPCs were assigned a value of 1.0 for the empirical correction factor for above-ground produce.

Metabolism Factor. Though not presented in Table F-8, the metabolism factor, MF , is a chemical-specific value used in calculations in the MPHRA. The HHRAP (USEPA, 2005) recommends that the metabolism factor be assigned a value of 0.01 (dimensionless) for bis(2-ethylhexyl)phthalate (BEHP) and a value of 1.0 (dimensionless) for all other compounds. Since BEHP is not a COPC evaluated under the MPHRA, all COPCs were assigned a value of 1.0 (dimensionless) for the metabolism factor.

F.4.3 Dermal Contact Parameters

Dermal contact parameters are chemical-specific values used to evaluate COPC uptake through contact with COPC-containing surface water and soil. The HHRAP (USEPA, 2005) does not contain chemical-specific parameters required for dermal exposure assessment. Therefore, the required parameters were either obtained directly from or calculated by the methodology presented in *Risk Assessment Guidance for Superfund (RAGS) Volume 1: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*. Office of Solid Waste and Emergency Response, Washington, D.C., EPA/540/R/99/005, July 2004 (RAGS, Part E) (USEPA, 2004). Table F-9 presents the chemical-specific dermal parameters used in this MPHRA.

Dermal Permeability Coefficient in Water. When measured or predicted values of the permeability coefficient of the chemical in water were unavailable in RAGS, Part E (USEPA, 2004), the coefficient was estimated using the empirical predictive correlation for permeability coefficient of organics (Equation 3-8 from RAGS, Part E (USEPA, 2004)), presented as Equation F-22 below:

$$\log K_p = -2.80 + 0.66 \log K_{ow} - 0.0056MW \quad \text{Eq. F-22}$$

where

- | | | |
|----------|---|---|
| K_p | = | dermal permeability coefficient of the chemical in water (cm/hr) |
| K_{ow} | = | octanol/water partition coefficient of the nonionized species (dimensionless) |
| MW | = | molecular weight (g/mole) |

Table F-9. Chemical-specific Dermal Parameters

COPC	Permeability Coefficient in Water	Dimensionless Ratio of the Permeability Coefficient through the Stratum Corneum Relative to the Permeability Coefficient across the Viable Epidermis ^d	Effective Diffusion Coefficient for Chemical Transfer through the Stratum Corneum ^e	Lag Time per Event ^f	Correlation Coefficient b ^g	Correlation Coefficient c ^h	Time to Reach Steady-State ⁱ
	(cm/hr)	(dimensionless)	(cm ² /hr)	(hr/event)	(dimensionless)	(dimensionless)	(hr)
	<i>K_p</i>	<i>B</i>	<i>D_{sc}</i>	<i>t_{event}</i>	<i>b</i>	<i>c</i>	<i>t</i>
1,1,1,2-tetrachloroethane	0.0182 ^b	0.0907	1.82E-07	0.916	NA	NA	2.20
1,1,1-trichloroethane	0.013 ^a	0.0577	2.84E-07	0.587	NA	NA	1.41
1,1,2,2-tetrachloroethane	0.0069 ^a	0.0344	1.82E-07	0.916	NA	NA	2.20
1,1-dichloroethane	0.0067 ^a	0.0256	4.42E-07	0.377	NA	NA	0.90
1,1-dichloroethene	0.012 ^a	0.0459	4.42E-07	0.377	NA	NA	0.90
1,2,3-trichlorobenzene	0.0719 ^b	0.3726	1.53E-07	1.091	NA	NA	2.62
1,2,4-trichlorobenzene	0.066 ^a	0.3419	1.53E-07	1.091	NA	NA	2.62
1,2,4-trimethyl benzene	0.0837	0.3529	3.36E-07	0.495	NA	NA	1.19
1,2-bis(ethylthio)-ethene	0.0184 ^b	0.0860	2.34E-07	0.712	NA	NA	1.71
1,2-bis(vinylthio)-ethane	0.017 ^b	0.0812	2.40E-07	0.694	NA	NA	1.66
1,2-dichlorobenzene	0.0405 ^b	0.1889	2.38E-07	0.700	NA	NA	1.68
1,2-dichlorobutane	0.0198 ^b	0.0859	3.08E-07	0.541	NA	NA	1.30
1,2-dichloroethane	0.0042 ^a	0.0161	4.42E-07	0.377	NA	NA	0.90
1,2-dichloropropane	0.0078 ^a	0.0319	3.69E-07	0.451	NA	NA	1.08
1,3-dichlorobenzene	0.0566 ^b	0.2639	2.38E-07	0.700	NA	NA	1.68
1,4-dichlorobenzene	0.042 ^a	0.1959	2.38E-07	0.700	NA	NA	1.68
1,4-dioxane	0.00033 ^a	0.0012	5.09E-07	0.328	NA	NA	0.79
1,4-dithiane	0.00274 ^b	0.0115	3.36E-07	0.496	NA	NA	1.19
1,4-oxathiane	0.000926 ^b	0.0036	4.14E-07	0.403	NA	NA	0.97
1-chlorobutane	0.0265 ^b	0.0982	4.80E-07	0.347	NA	NA	0.83
1-hexene	0.0925 ^b	0.3263	5.35E-07	0.311	NA	NA	0.75
2,2-dimethyl-trans-thiirane	0.00653 ^b	0.0236	5.08E-07	0.328	NA	NA	0.79
2,3-dimethyl-thiophene	0.0311 ^b	0.1266	3.73E-07	0.447	NA	NA	1.07
2,4,6-trinitrotoluene	0.000964 ^b	0.0056	8.47E-08	1.967	NA	NA	4.72
2,4-dichlorophenol	0.0159 ^b	0.0780	1.94E-07	0.860	NA	NA	2.06
2,4-dinitrotoluene	0.0031 ^a	0.0161	1.51E-07	1.101	NA	NA	2.64

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Table F-9. Chemical-specific Dermal Parameters (continued)

COPC	Permeability Coefficient in Water	Dimensionless Ratio of the Permeability Coefficient through the Stratum Corneum Relative to the Permeability Coefficient across the Viable Epidermis ^d	Effective Diffusion Coefficient for Chemical Transfer through the Stratum Corneum ^e	Lag Time per Event ^f	Correlation Coefficient b ^g	Correlation Coefficient c ^h	Time to Reach Steady-State
	(cm/hr)	(dimensionless)	(cm ² /hr)	(hr/event)	(dimensionless)	(dimensionless)	(hr)
	<i>K_p</i>	<i>B</i>	<i>D_{sc}</i>	<i>t_{event}</i>	<i>b</i>	<i>c</i>	<i>t</i>
2,6-dinitrotoluene	0.0021 ^a	0.0109	1.51E-07	1.102	NA	NA	2.64
2-butanone	0.00096 ^a	0.0031	6.25E-07	0.266	NA	NA	0.64
2-chlorobutane	0.0166 ^b	0.0613	4.80E-07	0.347	NA	NA	0.83
2-chloroethoxyethane	0.000994 ^b	0.0052	1.42E-07	1.173	NA	NA	2.82
2-ethyl 1,3-butadiene	0.0584 ^b	0.2035	5.50E-07	0.303	NA	NA	0.73
2-hexanone	0.00355 ^b	0.0137	4.36E-07	0.383	NA	NA	0.92
2-methyl phenol	0.016 ^c	0.0642	3.89E-07	0.428	NA	NA	1.03
2-methyl-1,3-dithiacyclopentane	0.00818 ^b	0.0345	3.36E-07	0.495	NA	NA	1.19
2-methyl-1,3-dithiane	0.0146 ^b	0.0650	2.80E-07	0.594	NA	NA	1.43
2-methyl-1,3-oxathiolane	0.000832 ^b	0.0033	4.14E-07	0.403	NA	NA	0.97
2-methylnaphthalene	0.0894 ^b	0.4100	2.53E-07	0.658	NA	NA	1.58
3-methyl phenol	0.015 ^c	0.0600	3.93E-07	0.424	NA	NA	1.02
4-methyl phenol	0.018 ^c	0.0720	3.93E-07	0.424	NA	NA	1.02
4-methyl-2-pentanone	0.0027 ^a	0.0104	4.36E-07	0.383	NA	NA	0.92
acenaphthylene	0.0887 ^b	0.4211	2.23E-07	0.748	NA	NA	1.80
acetaldehyde	0.00063 ^a	0.0016	8.98E-07	0.186	NA	NA	0.45
acetone	0.000520 ^b	0.0015	7.49E-07	0.222	NA	NA	0.53
acetylene	0.00199 ^b	0.0039	1.13E-06	0.147	NA	NA	0.35
acrolein	0.00065 ^a	0.0019	7.69E-07	0.217	NA	NA	0.52
alpha-methylstyrene	0.0685 ^b	0.2864	3.46E-07	0.482	NA	NA	1.16
benzene	0.015 ^a	0.0510	5.79E-07	0.288	NA	NA	0.69
bis(2-chloroisopropyl) ether	0.00911 ^b	0.0458	1.75E-07	0.955	NA	NA	2.29
carbon disulfide	0.017 ^a	0.0570	5.94E-07	0.281	NA	NA	0.67
chlorobenzene	0.028 ^a	0.1143	3.71E-07	0.449	NA	NA	1.08
chloroethane	0.0061 ^a	0.0188	6.90E-07	0.242	NA	NA	0.58
chloroform	0.0068 ^a	0.0286	3.40E-07	0.490	NA	NA	1.18
chloromethane	0.0033 ^a	0.0090	8.27E-07	0.202	NA	NA	0.48
chloromethoxyethane	0.00160 ^b	0.0060	4.68E-07	0.356	NA	NA	0.85
cis-1,2-dichloroethene	0.00815 ^b	0.0309	4.54E-07	0.367	NA	NA	0.88

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Table F-9. Chemical-specific Dermal Parameters (continued)

COPC	Permeability Coefficient in Water	Dimensionless Ratio of the Permeability Coefficient through the Stratum Corneum Relative to the Permeability Coefficient across the Viable Epidermis ^d	Effective Diffusion Coefficient for Chemical Transfer through the Stratum Corneum ^e	Lag Time per Event ^f	Correlation Coefficient b ^g	Correlation Coefficient c ^h	Time to Reach Steady-State
	(cm/hr)	(dimensionless)	(cm ² /hr)	(hr/event)	(dimensionless)	(dimensionless)	(hr)
	<i>K_p</i>	<i>B</i>	<i>D_{sc}</i>	<i>t_{event}</i>	<i>b</i>	<i>c</i>	<i>t</i>
dichlorodifluoromethane	0.009 ^a	0.0381	3.33E-07	0.500	NA	NA	1.20
diethyl ether	0.016 ^c	0.0530	6.09E-07	0.273	NA	NA	0.66
diethyl phthalate	0.0039 ^a	0.0224	9.03E-08	1.847	NA	NA	4.43
di-n-butyl phthalate	0.0554 ^b	0.3553	4.38E-08	3.807	NA	NA	9.14
diphenylamine	0.0365 ^b	0.1826	1.79E-07	0.932	NA	NA	2.24
ethane	0.0168 ^b	0.0355	1.08E-06	0.155	NA	NA	0.37
ethanol	0.000546 ^b	0.0014	8.75E-07	0.190	NA	NA	0.46
ethene	0.00614 ^b	0.0125	1.10E-06	0.151	NA	NA	0.36
ethyl centralite	0.0295 ^b	0.1856	4.98E-08	3.347	NA	NA	8.03
ethylbenzene	0.049 ^a	0.1942	4.03E-07	0.414	NA	NA	0.99
HD	0.0045 ^a	0.0218	2.04E-07	0.818	NA	NA	1.96
hexachlorobutadiene	0.081 ^a	0.5031	5.49E-08	3.035	NA	NA	7.28
hexachloroethane	0.03 ^a	0.1775	7.49E-08	2.226	NA	NA	5.34
hexane	0.196 ^b	0.6983	5.22E-07	0.320	0.9416161	0.894600649	1.24
methane	0.006750	0.0104	1.29E-06	0.129	NA	NA	0.31
methyl tert-butyl ether	0.00212 ^b	0.0077	5.08E-07	0.328	NA	NA	0.79
methylene chloride	0.0035 ^a	0.0124	5.30E-07	0.314	NA	NA	0.75
monoethanolamine	9.85 ^b	0.0003	7.21E-07	0.231	NA	NA	0.55
naphthalene	0.047 ^a	0.2047	3.04E-07	0.549	NA	NA	1.32
nitrobenzene	0.00539 ^b	0.0230	3.24E-07	0.514	NA	NA	1.23
nitroglycerin	0.000841 ^b	0.0049	8.48E-08	1.966	NA	NA	4.72
octane	0.953 ^b	3.9187	3.63E-07	0.459	11.41555159	3.986448002	1.98
pentane	0.108 ^b	0.3527	6.25E-07	0.267	NA	NA	0.64
phenanthrene	0.149 ^b	0.7628	1.59E-07	1.047	1.026431754	0.951927413	4.04
phenol	0.00460 ^b	0.0172	4.71E-07	0.354	NA	NA	0.85
propene	0.0136 ^b	0.0339	9.21E-07	0.181	NA	NA	0.43
styrene	0.037 ^a	0.1452	4.14E-07	0.403	NA	NA	0.97
tert-butyl alcohol	0.00104 ^b	0.0034	6.10E-07	0.273	NA	NA	0.66
tetracene	0.529 ^b	3.0722	8.35E-08	1.997	7.402789899	3.154032346	8.45
tetrachloroethene	0.033 ^a	0.1634	1.87E-07	0.892	NA	NA	2.14
tetryl	0.000472 ^b	0.0031	3.91E-08	4.265	NA	NA	10.24

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Table F-9. Chemical-specific Dermal Parameters (continued)

COPC	Permeability Coefficient in Water	Dimensionless Ratio of the Permeability Coefficient through the Stratum Corneum Relative to the Permeability Coefficient across the Viable Epidermis ^d	Effective Diffusion Coefficient for Chemical Transfer through the Stratum Corneum ^e	Lag Time per Event ^f	Correlation Coefficient b^g	Correlation Coefficient c^h	Time to Reach Steady-State
	(cm/hr)	(dimensionless)	(cm ² /hr)	(hr/event)	(dimensionless)	(dimensionless)	(hr)
	K_p	B	D_{sc}	τ_{event}	b	c	t
thiirane	0.00250 ^b	0.0075	7.30E-07	0.228	NA	NA	0.55
thiodiglycol	0.000126 ^b	0.0005	3.28E-07	0.508	NA	NA	1.22
toluene	0.031 ^a	0.1144	4.83E-07	0.345	NA	NA	0.83
trans-1,2-dichloroethene	0.0110 ^b	0.0418	4.54E-07	0.367	NA	NA	0.88
trichloroethene	0.012 ^a	0.0529	2.91E-07	0.572	NA	NA	1.37
vinyl chloride	0.0056 ^a	0.0170	7.08E-07	0.235	NA	NA	0.57
xylenes	0.053 ^a	0.2100	4.03E-07	0.413	NA	NA	0.99
aluminum	0.00185 ^b	0.0037	1.12E-06	0.149	NA	NA	0.36
ammonia	0.00181 ^b	0.0029	1.27E-06	0.131	NA	NA	0.31
arsenic	0.001 ^a	0.0033	6.03E-07	0.276	NA	NA	0.66
cadmium	0.001 ^a	0.0041	3.72E-07	0.448	NA	NA	1.08
chlorine	0.00231 ^b	0.0075	6.35E-07	0.262	NA	NA	0.63
copper	0.001 ^a	0.0031	6.99E-07	0.238	NA	NA	0.57
hydrogen chloride	0.00225 ^b	0.0052	9.90E-07	0.168	NA	NA	0.40
hydrogen cyanide	0.000765 ^b	0.0015	1.12E-06	0.149	NA	NA	0.36
lead	0.000332 ^b	0.0018	1.10E-07	1.521	NA	NA	3.65
nickel	0.002 ^c	0.0059	7.43E-07	0.224	NA	NA	0.54
silver	0.0006 ^c	0.0024	3.94E-07	0.423	NA	NA	1.01

- a. Predicted value of K_p presented as Exhibit B-2 in RAGS, Part E (USEPA, 2004).
 - b. Calculated using Equation 3-8 of RAGS, Part E (USEPA, 2004).
 - c. Measured value of K_p presented as Exhibit B-1 in RAGS, Part E (USEPA, 2004).
 - d. Calculated using Equation A.1 of RAGS, Part E (USEPA, 2004).
 - e. Calculated using Equation A.2 of RAGS, Part E (USEPA, 2004).
 - f. Calculated using Equation A.4 of RAGS, Part E (USEPA, 2004).
 - g. Calculated using Equation A.7 of RAGS, Part E (USEPA, 2004).
 - h. Calculated using Equation A.8 of RAGS, Part E (USEPA, 2004).
 - i. Calculated using Equation A.5 of RAGS, Part E (USEPA, 2004).
 - j. Calculated using Equation A.6 of RAGS, Part E (USEPA, 2004).
- NA -Not applicable. B is less than 0.6; therefore, b and c do not require calculation.

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Dimensionless Ratio of the Permeability Coefficient through the Statum Corneum Relative to its Permeability Coefficient across the Viable Epidermis. The dimensionless ratio of the permeability coefficient through the statum corneum relative to the permeability coefficient across the viable epidermis (parameter B) was calculated for each compound using Equation A.1 from RAGS, Part E (USEPA, 2004), presented below as Equation F-23:

$$B = K_p \frac{\sqrt{MW}}{2.6} \quad \text{Eq. F-23}$$

where

- B = dimensionless ratio of the permeability coefficient of a compound through the statum corneum relative to its permeability coefficient across the viable epidermis (dimensionless)
- K_p = dermal permeability coefficient of the chemical in water (cm/hr)
- MW = molecular weight (g/mole)

Effective Diffusion Coefficient for Chemical Transfer through the Statum Corneum. The effective diffusion coefficient for chemical transfer through the statum corneum was calculated for each COPC using Equation A.2 from RAGS, Part E (USEPA, 2004) presented below as Equation F-24:

$$\log \frac{D_{sc}}{I_{sc}} = -2.80 - 0.0056MW \quad \text{Eq. F-24}$$

where

- D_{sc} = effective diffusion coefficient for chemical transfer through the statum corneum (cm²/hr)
- I_{sc} = thickness of the statum corneum (cm)
- MW = molecular weight of the compound (g/mole)

Lag Time per Event. The lag time per event was calculated for each COPC using Equation A.4 of RAGS, Part E (USEPA, 2004) presented below as Equation F-25:

$$\tau_{event} = \frac{I_{sc}^2}{6D_{sc}} \quad \text{Eq. F-25}$$

where

- τ_{event} = lag time per event (hr/event)
- D_{sc} = effective diffusion coefficient for chemical transfer through the statum corneum (cm²/hr)
- I_{sc} = thickness of the statum corneum (cm)

Time to Reach Steady-state. The time to reach steady-state was calculated using either Equation A.5 or Equation A.6 from RAGS, Part E (USEPA, 2004), depending on the magnitude of the dimensionless ratio of the permeability coefficient of the compound through the statum corneum relative to its permeability coefficient across the viable epidermis (parameter B).

When parameter B is less than or equal to 0.6, the time to reach steady-state was calculated using Equation A.5 from RAGS, Part E (USEPA, 2004), presented below as Equation F-26:

$$t^* = 2.4\tau_{event} \quad \text{Eq. F-26}$$

where

$$\begin{aligned} t^* &= \text{time to reach steady-state (hr)} \\ \tau_{event} &= \text{lag time per event (hr/event)} \end{aligned}$$

When parameter B is greater than 0.6, the time to reach steady-state was calculated using Equation A.6 from RAGS, Part E (USEPA, 2004), presented below as Equation F-27:

$$t^* = 6\tau_{event} \left(b - \sqrt{b^2 - c^2} \right) \quad \text{Eq. F-27}$$

where

$$\begin{aligned} t^* &= \text{time to reach steady-state (hr)} \\ \tau_{event} &= \text{lag time per event (hr/event)} \\ b &= \text{correlation coefficient } b \text{ (dimensionless)} \\ c &= \text{correlation coefficient } c \text{ (dimensionless)} \end{aligned}$$

The correlation coefficients b and c used in Equation F-27 were calculated using Equation A.7 and Equation A.8 from RAGS, Part E (USEPA, 2004), respectively, and are presented below as Equation F-28 and Equation F-29, respectively:

$$b = \frac{2(1+B)^2}{\pi} - c \quad \text{Eq. F-28}$$

where

$$\begin{aligned} b &= \text{correlation coefficient } b \text{ (dimensionless)} \\ B &= \text{dimensionless ratio of the permeability coefficient of a compound through the statum corneum relative to its permeability coefficient across the viable epidermis (dimensionless)} \\ c &= \text{correlation coefficient } c \text{ (dimensionless)} \end{aligned}$$

$$c = \frac{1 + 3B + 3B^2}{3(1+B)} \quad \text{Eq. F-29}$$

where

$$\begin{aligned} c &= \text{correlation coefficient } c \text{ (dimensionless)} \\ B &= \text{dimensionless ratio of the permeability coefficient of a compound through the statum corneum relative to its permeability coefficient across the viable epidermis (dimensionless)} \end{aligned}$$

Dermal Absorption Fraction from Soil. All COPCs evaluated for dermal absorption from soil in this MPHRA were assigned a value of 0.1 (dimensionless) for the dermal adsorption fraction from soil. This value is provided by Exhibit 3-4 of RAGS, Part E (USEPA, 2004) for semi-volatile organic compounds.

Fraction of Contaminant Absorbed in the Gastrointestinal Tract. With the exception of cadmium, nickel, and silver, all COPCs evaluated for dermal absorption from soil and water in this MPHRA were assigned a value of 1.0 (dimensionless) for the fraction of contaminant absorbed in the gastrointestinal tract. For cadmium, nickel, and silver, the fraction of contaminant absorbed by the gastrointestinal tract were assigned values of 0.025, 0.04, and 0.04, respectively. Values for all COPCs are provided by Exhibit 4-1 of RAGS, Part E (USEPA, 2004)

F.4.4 Cuticular Resistance for Individual Leaves to Uptake by Lipids

The cuticular resistance for individual leaves to uptake by lipids, r_{cl} , represents the chemical-specific resistance to uptake by individual leaves in a vegetative canopy and is a necessary input for air dispersion modeling of vapor-phase COPCs using AERMOD. Values for r_{cl} were obtained from or calculated using the procedures set out in *Deposition Parameterizations for the Industrial Source Complex (ISC3) Model* (Wesely et al., 2002). Table F-10 presents the r_{cl} values used in the MPHRA, as well as all of the intermediate parameters calculated and used in the calculation of r_{cl} . Rows that are shaded gray in Table F-10 indicate that the value for r_{cl} was provided in Wesley et al, and the calculation for r_{cl} was not required.

Cuticle-Water Partition Coefficient. The cuticle-water partition coefficient is calculated using two separate methods: one for semi-volatile compounds and other compounds with saturation vapor pressures less than 125 Pa; and the second for volatile organic compounds and other compounds with saturation vapor pressure greater than 125 Pa.

For compounds with saturation vapor pressures less than 125 Pa, the cuticle-water partition coefficient was calculated using Equation 36a from *Deposition Parameterizations for the ISC3 Model* (Wesely et al., 2002), presented as Equation F-30 below:

$$\log K_{cw} = 0.973 \log K_{ow} + 0.045 \quad \text{Eq. F-30}$$

where

$$\begin{aligned} K_{cw} &= \text{cuticle-water partition coefficient (dimensionless)} \\ \log K_{ow} &= \text{log of the octanol-water partition coefficient (dimensionless)} \end{aligned}$$

For compounds with saturation vapor pressures greater than 125 Pa, the cuticle-water partition coefficient was calculated using the following procedure: calculate the cuticle-air partition coefficient using Equation 6 from *Sorption of Volatile Organic Chemicals in Plant Surfaces* (Welke et al., 1998), presented as Equation F-31 below; then calculate the cuticle-water partition coefficient using Equation 37b from *Deposition Parameterizations for the ISC3 Model* (Wesely et al., 2002), presented as Equation F-32 below:

$$\log K_{ca} = 6.290 - 0.892 \log V_p \quad \text{Eq. F-31}$$

where

$$\begin{aligned} K_{ca} &= \text{cuticle-air partition coefficient (dimensionless)} \\ V_p &= \text{vapor pressure (Pa)} \end{aligned}$$

$$K_{cw} = \frac{K_{ca}H}{RT_a} \quad \text{Eq. F-32}$$

where

- K_{cw} = cuticle-water partition coefficient (dimensionless)
- K_{ca} = cuticle-air partition coefficient (dimensionless)
- H = Henry's Law Constant (atm-m³/mol)
- R = universal gas constant (8.205 x 10⁻⁵ atm-m³/mol-K)
- T_a = ambient air temperature (298 K)

Table F-10. Derivation of Cuticular Resistance for Individual Leaves to Uptake by Lipids

COPC	Log of the Cuticle-Air Partition Coefficient ^a	Log of the Cuticle-Water Partition Coefficient	Molar Volume of the Liquid Chemical at the Normal Boiling Point ^d	Log of the Aqueous Phase Permeance Coefficient ^e	Gaseous Phase Permeance Coefficient ^f	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^g
	log K _{ca}	log K _{cw}	V _m	log P _{cw}	P _{ca}	r _{cl}
	(dimensionless)	(dimensionless)	(cm ³ /mol)	(dimensionless)	(m/s)	(s/cm)
1,1,1,2-tetrachloroethane	3.43	2.43	135.4	-8.21	3.87E-07	2.59E+04
1,1,1-trichloroethane						8.15E+04
1,1,1,2,2-tetrachloroethane						4.95E+04
1,1-dichloroethane						1.16E+05
1,1-dichloroethene						5.78E+04
1,2,3-trichlorobenzene	NA	3.99	158.7	-6.50	3.84E-05	2.60E+02
1,2,4-trichlorobenzene						4.82E+02
1,2,4-trimethyl benzene						1.30E+04
1,2-bis(ethylthio)-ethene	NA	2.84	100	-5.73	2.06E-03	4.85E+00
1,2-bis(vinylthio)-ethane	NA	2.79	100	-5.84	2.53E-03	3.95E+00
1,2-dichlorobenzene	4.28	3.17	137.8	-7.01	7.82E-06	1.28E+03
1,2-dichlorobutane	3.22	3.16	138	-7.03	6.64E-07	1.51E+04
1,2-dichloroethane						1.31E+05
1,2-dichloropropane	2.86	1.92	115.8	-8.53	1.62E-07	6.18E+04
1,3-dichlorobenzene	NA	3.55	137.8	-6.35	2.19E-05	4.57E+02
1,4-dichlorobenzene						5.04E+02
1,4-dioxane	2.98	-0.72	93.6	-14.32	1.53E-10	6.52E+07
1,4-dithiane	4.22	0.52	125	-11.48	1.02E-07	9.81E+04
1,4-oxathiane	3.80	0.15	136.6	-12.23	1.68E-08	5.94E+05
1-chlorobutane	2.61	2.44	117.1	-7.52	2.77E-07	3.61E+04
1-hexene	2.37	3.60	133.2	-6.05	3.34E-07	3.00E+04
2,2-dimethyl-trans-thiirane	NA	1.68	100	-8.48	8.24E-07	1.21E+04
2,3-dimethyl-thiophene	3.71	2.87	144	-7.74	7.87E-07	1.27E+04
2,4,6-trinitrotoluene	NA	1.60	166.5	-10.19	2.02E-03	4.94E+00
2,4-dichlorophenol	NA	2.87	160.2	-8.22	2.87E-04	3.48E+01
2,4-dinitrotoluene	NA	1.97	165	-9.64	3.81E-04	2.62E+01
2,6-dinitrotoluene	NA	1.72	165	-10.00	2.04E-05	4.90E+02
2-butanone						3.88E+07
2-chlorobutane	2.44	2.43	117.1	-7.54	1.82E-07	5.49E+04
2-chloroethoxyethane	NA	1.29	124.5	-10.01	1.90E-05	5.27E+02
2-ethyl 1,3-butadiene	2.53	3.53	125.8	-5.80	9.86E-07	1.01E+04
2-hexanone	3.45	1.03	140.6	-10.74	2.96E-08	3.37E+05

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Table F-10. Derivation of Cuticular Resistance for Individual Leaves to Uptake by Lipids (continued)

COPC	Log of the Cuticle-Air Partition Coefficient ^a	Log of the Cuticle-Water Partition Coefficient	Molar Volume of the Liquid Chemical at the Normal Boiling Point ^d	Log of the Aqueous Phase Permeance Coefficient ^e	Gaseous Phase Permeance Coefficient ^f	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^g
	log K _{ca}	log K _{cw}	V _m	log P _{cw}	P _{ca}	r _{cl}
	(dimensionless)	(dimensionless)	(cm ³ /mol)	(dimensionless)	(m/s)	(s/cm)
2-methyl phenol						5.58E+01
2-methyl-1,3-dithiacyclopentane	4.07	0.37	140	-11.85	4.44E-08	2.25E+05
2-methyl-1,3-dithiane	NA	2.57	143	-8.19	1.50E-04	6.67E+01
2-methyl-1,3-oxathiolane	NA	0.49	100	-11.31	1.40E-07	7.15E+04
2-methylnaphthalene						4.71E+02
3-methyl phenol						3.27E+01
4-methyl phenol						2.54E+01
4-methyl-2-pentanone						8.24E+05
acenaphthylene						3.59E+01
acetaldehyde						1.50E+11
acetone	2.29	-0.51	74	-14.12	2.98E-11	3.36E+08
acetylene	0.29	0.23	37	-10.98	7.45E-11	1.34E+08
acrolein						5.80E+05
alpha-methylstyrene	4.15	3.16	155.2	-7.63	1.41E-06	7.08E+03
benzene						2.51E+04
bis(2-chloroisopropyl) ether	NA	2.58	189.8	-9.25	9.35E-08	1.07E+05
carbon disulfide						7.45E+02
chlorobenzene						6.02E+03
chloroethane						2.11E+04
chloroform						1.62E+05
chloromethane						1.89E+06
chloromethoxyethane	2.81	1.03	102.3	-10.08	3.15E-08	3.17E+05
cis-1,2-dichloroethene	2.34	1.57	86.2	-8.15	2.61E-07	3.83E+04
dichlorodifluoromethane	1.11	2.25	114.7	-7.80	7.01E-09	1.43E+06
diethyl ether	1.96	-0.01	106.1	-12.49	1.85E-10	5.41E+07
diethyl phthalate	NA	2.48	259	-10.20	2.13E-05	4.70E+02
di-n-butyl phthalate						6.46E+01
diphenylamine	NA	3.45	228.8	-8.89	7.31E-05	1.37E+02
ethane	0.38	1.69	51.8	-4.70	6.06E-06	1.65E+03
ethanol	2.81	-0.88	59.2	-16.00	3.04E-12	3.29E+09
ethene	0.19	1.16	44.4	-6.28	3.52E-07	2.84E+04
ethyl centralite	NA	4.13	354.9	-9.71	3.63E-04	2.75E+01
ethylbenzene						1.65E+04
HD	NA	2.39	163.6	-9.00	4.60E-06	2.18E+03

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Table F-10. Derivation of Cuticular Resistance for Individual Leaves to Uptake by Lipids (continued)

COPC	Log of the Cuticle-Air Partition Coefficient ^a	Log of the Cuticle-Water Partition Coefficient	Molar Volume of the Liquid Chemical at the Normal Boiling Point ^d	Log of the Aqueous Phase Permeance Coefficient ^e	Gaseous Phase Permeance Coefficient ^f	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^g
	log K _{ca}	log K _{cw}	V _m	log P _{cw}	P _{ca}	r _{cl}
	(dimensionless)	(dimensionless)	(cm ³ /mol)	(dimensionless)	(m/s)	(s/cm)
hexachlorobutadiene						1.45E+04
hexachloroethane						2.94E+03
hexane						2.73E+04
methane	-0.66	0.77	29.6	-6.30	1.16E-07	8.64E+04
methyl tert-butyl ether						1.11E+07
methylene chloride						9.07E+04
monoethanolamine	NA	-1.23	73.4	-16.47	1.60E-10	6.23E+07
naphthalene						3.65E+02
nitrobenzene						7.51E+02
nitroglycerin	NA	1.51	161	-10.24	3.45E-03	2.90E+00
octane	3.37	5.49	185	-5.42	1.81E-07	5.53E+04
pentane	1.98	3.69	118.4	-5.07	1.03E-06	9.67E+03
phenanthrene						2.33E+01
phenol						3.33E+01
propene	0.88	1.78	66.6	-6.10	6.17E-07	1.62E+04
styrene						1.13E+04
tert-butyl alcohol	2.96	-0.47	103.6	-13.57	4.58E-10	2.18E+07
tetracene						3.39E-02
tetrachloroethene						6.04E+03
tetryl	NA	1.64	241	-10.86	7.79E-04	1.28E+01
thiirane	2.26	0.41	70	-11.10	3.52E-09	2.84E+06
thiodiglycol	NA	-0.57	136.6	-13.47	2.80E-06	3.57E+03
toluene						1.74E+04
trans-1,2-dichloroethene	2.15	1.73	86.2	-7.69	3.28E-07	3.05E+04
trichloroethene						1.88E+04
vinyl chloride						7.35E+03
xylenes						2.00E+04
aluminum	Particle-phase COPC					
ammonia	0.94	-2.24	100	-17.82	1.40E-14	6.97E+11
arsenic	Particle-phase COPC					
cadmium	Particle-phase COPC					
chlorine	1.04	0.72	49.2	-9.02	1.25E-08	8.00E+05
copper	Particle-phase COPC					
hydrogen chloride	0.34	-0.16	28.3	-13.85	2.76E-13	3.62E+10

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Table F-10. Derivation of Cuticular Resistance for Individual Leaves to Uptake by Lipids (continued)

COPC	Log of the Cuticle-Air Partition Coefficient ^a	Log of the Cuticle-Water Partition Coefficient	Molar Volume of the Liquid Chemical at the Normal Boiling Point ^d	Log of the Aqueous Phase Permeance Coefficient ^e	Gaseous Phase Permeance Coefficient ^f	Cuticular Resistance for Individual Leaves to Uptake by Lipids ^g
	log K _{ca}	log K _{cw}	V _m	log P _{cw}	P _{ca}	r _{cl}
	(dimensionless)	(dimensionless)	(cm ³ /mol)	(dimensionless)	(m/s)	(s/cm)
hydrogen cyanide	1.83	-0.43	34.1	-15.48	3.78E-13	9.01E+12
lead	Particle-phase COPC					
nickel	Particle-phase COPC					
silver	Particle-phase COPC					

NA - not appropriate. Log K_{ca} is not needed to calculate r_{cl} for this compound.

- a. Calculated using Equation 6 of Welke et al., 1998 for compounds with vapor pressures greater than 125 Pa.
- b. Calculated using Equation 37b of Wesely et al., 2002, for compounds with V_p > 125 Pa.
- c. Calculated using Equation 36a of Wesely et al., 2002, for compounds with V_p < 125 Pa.
- d. Estimated using Le Bas estimation Method described in Wesely et al., 2002.
- e. Calculated using Equation 36b of Wesely et al., 2002.
- f. $P_{ca} = P_{cw}(H/RT_a)(2.5/1.0)^2$ as described on page 26 of Wesely et al, 2002.
- g. $R_{cl} = 1/P_{ca}(1/100)$ as described on page 26 of Wesely et al., 2002.

Molar Volume of the Liquid Chemical at the Normal Boiling Point. The molar volume of the liquid chemical at the normal boiling point was evaluated as described in *Deposition Parameterizations for the ISC3 Model* (Wesely et al., 2002) using the Le Bas Estimation Method. For each atom in a compound, an incremental volume is assigned based on the type of atom and its bonding within the compound. The molar volume is the summation of the volume increments for each individual atom in a compound.

Aqueous Phase Permeance Coefficient. The aqueous phase permeance coefficient was calculated using Equation 36b from *Deposition Parameterizations for the ISC3 Model* (Wesely et al., 2002), presented as Equation F-33 below:

$$\log P_{cw} = \frac{238 \log K_{cw}}{V_m} - 12.48 \quad \text{Eq. F-33}$$

where

P_{cw}	=	aqueous phase permeance coefficient (m/sec)
K_{cw}	=	cuticle-water partition coefficient (dimensionless)
V_m	=	molar volume of the liquid chemical at the normal boiling point (cm ³ /mol)

Gaseous Phase Permeance Coefficient. The gaseous phase permeance coefficient was calculated as described in *Deposition Parameterizations for the ISC3 Model* (Wesely et al., 2002) and is presented as Equation F-34 below:

$$P_{ca} = \frac{P_{cw}RT_a}{H} \left(\frac{2.5}{1.0} \right)^2 \quad \text{Eq. F-34}$$

where

P_{ca}	=	gaseous phase permeance coefficient (m/sec)
P_{cw}	=	aqueous phase permeance coefficient (m/sec)
H	=	Henry's Law Constant (atm-m ³ /mol)
R	=	universal gas constant (8.205 x 10 ⁻⁵ atm-m ³ /mol-K)
T_a	=	ambient air temperature (298 K)
$(2.5/1.0)^2$	=	adjustment factor to change membrane thickness from 2.5 μm to 1.0 μm (dimensionless)

Cuticular Resistance for Individual Leaves to Uptake by Lipids. The cuticular resistance for individual leaves to uptake by lipids was calculated as described in *Deposition Parameterizations for the ISC3 Model* (Wesely et al., 2002) and is presented as Equation F-35 below:

$$r_{cl} = \frac{1}{P_{ca}} \left(\frac{1}{100} \right) \quad \text{Eq. F-35}$$

where

r_{cl}	=	cuticular resistance for individual leaves to uptake by lipids (s/cm)
P_{ca}	=	gaseous phase permeance coefficient (m/s)
$(1/100)$	=	conversion factor (m/cm)

F.4.5 Breast Milk Pathway Parameters

Average Maternal Intake of COPC. The average maternal intake of COPC (m) represents the average amount of each COPC ingested by the mother of the infant in each infant exposure scenario and is the sum of direct intake (via inhalation, calculated by Equation D-39 in Appendix D) and indirect intake (via ingestion and dermal absorption, calculated by Equation D-56 in Appendix D).

Fraction of Ingested Contaminant Which is Absorbed. The *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions* (USEPA, 1998) explains that the fraction of ingested contaminant that is absorbed (f_4) has been established for dioxin and dioxin-like PCBs as 0.9. However, for non-lipophilic compounds, all of the ingested contaminant is assumed to be absorbed (i.e., $f_4 = 1.0$).

Half Life of COPC in Adults. When selecting the half-life of a chemical in adults (h), the preferred value is one that is reported as the chemical half-life in the whole body or fat, in this order. These values are generally not available in literature. A literature search indicated that the half-life of benzene, toluene, and xylenes ranged from approximately 1 hour to 5 days (ATSDR; 2000, 2007a, 2007b). These values represented the upper range of half-life values for the majority of non-lipophilic organic compounds. A longer half-life leads to a greater breast milk concentration. Therefore, as a conservative assumption, a half-life of 5 days was used for all non-lipophilic organic COPCs for which the breast milk pathway was evaluated. A limited literature review conducted by Colorado Department of Public Health and Environment (CDPHE) indicated that, of the metal COPCs (i.e., aluminum, arsenic, cadmium, copper, lead and silver), whole-body half-life values in adults are available only for cadmium (26 years) and arsenic (44 days). Per direction of CDPHE, the 26-year half-life of cadmium was used as the default half-life for all metal COPCs without a specific value. The published 44-day half-life was used for arsenic.

Fraction of Ingested Chemical Stored in Fat and Stored in Blood Plasma. USEPA (1998) suggests that the fraction of ingested chemicals stored in maternal fat (f_f) can be greater than 90 percent. For these calculations, contaminants were assumed to partition into either maternal fat or maternal whole blood (i.e. the sum of the two partition fractions is 1.0). No data were found for the individual chemicals evaluated in this MPHRA, so a conservative value of 0.5 (50 percent) was used for f_f in all calculations. A sensitivity analysis indicated that the total concentration in milk increased as the fraction of chemical which partitioned into maternal whole blood increased. The fraction of ingested COPC stored in maternal blood plasma (f_{pl}) was calculated following guidance provided in (USEPA, 1998) using 0.5 as the fraction stored in maternal whole blood.

F.5 REFERENCES

- ATSDR, 2000. Toxicological Profile for Toluene. U.S. Department of Health and Human Services, Public Health Service, Atlanta, GA. September 2000.
- ATSDR, 2007a. Toxicological Profile for Benzene. U.S. Department of Health and Human Services, Public Health Service, Atlanta, GA. August 2007.
- ATSDR, 2007b. Toxicological Profile for Xylenes. U.S. Department of Health and Human Services, Public Health Service, Atlanta, GA. August 2007.
- Chafin, D.T., 1996. *Hydrogeology of the Alluvial Aquifers at the Pueblo Depot Activity Near Pueblo, Colorado*, Water Resources Investigation Report 95-4137, U.S. Geological Survey, Denver, CO.
- Junge, C.E., 1977. *Fate of Pollutants in the Air and Water Environments*, Part I; Suffet, I.H., Ed.; Wiley; New York.
- Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko, 1991. *Handbook of Environmental Degradation Rates*. Lewis Publishers. Chelsea, MI.
- Miller, D.W. 1963. *Water Atlas of the United States: Basic Facts about the Nation's Water Resources*. Water Information Center.
- Munro, N.B., Talmadge, S.S, Griffin, G.D., Waters, L.C., Watson, A.P., King, J.F., and Hauschild, V. 1999. "The Sources, Fate, and Toxicity of Chemical Warfare Agent Degradation Products," *Environmental Health Perspectives*, Volume 107, Number 12.
- National Oceanic and Atmospheric Administration (NOAA), 2004. Climatography of the United States No. 81: Monthly Station Normals of Temperature, Precipitation, and Heating and Cooling Degree Days 1971-2000. 05 Colorado. National Environmental Satellite, Data, and Information Service, National Climatic Data Center. Asheville, NC, February 2004. (Online address: <http://cdo.ncdc.noaa.gov/climatenormals/clim81/COnorm.pdf>)
- National Resource Conservation Service (NRCS), 2006. Revised Universal Soil Loss Equation software package, RUSLE2. May 2006.
- SAIC, 2006. *Draft Final Munitions Analysis and Characterization Report*, compiled for US Army PCD, May 2006.
- Syracuse Research Corporation, 2003a. PHYSPROP Database. (Available online at <http://www.syrres.com/esc/physdemo.htm>)
- Syracuse Research Corporation, 2003b. CHEMFATE Database.
- US Army, 2002. Program Manager for Chemical Demilitarization. *Destruction of Chemical Munitions at Pueblo Chemical Depot, Colorado Final Environmental Impact Statement*. March 2002.

USEPA, 1989. *Risk Assessment Guidance for Superfund, Volume I, Human Health Evaluation Manual (Part A)*. Interim Final. Office of Emergency and Remedial Response. EPA/504/1-89/002.

USEPA, 1994. *Air Emissions Model for Waste and Wastewater*. Office of Air Quality Planning and Standards, Research Triangle Park, NC. EPA-453/R-94-080A, November 1994.

USEPA, 1998. *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions*. National Center for Environmental Assessment, Washington, DC. EPA 600/R-98/137.

USEPA, 2000-2007. Estimation Program Interface (EPI) Suite. Copyright © 2000-2007. Available online at <http://www.epa.gov/oppt/exposure/pubs/episuitedi.htm>

USEPA, 2002. *Estimated Per Capita Fish Consumption in the United States*. Washington, DC. EPA-821-C-02-003, August 2002.

USEPA, 2004. *Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)*. Office of Superfund Remediation and Technology Innovation, Washington, DC. EPA/540/R/99/005.

USEPA, 2005. *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities*. Office of Solid Waste and Emergency Response, Washington, DC. EPA-530-R-05-006, September 2005.

USEPA, 2011. Exposure Factors Handbook. EPA/600/R-09/052F, September 2011.

Welke, B., K. Ettliger, and M. Riederer, 1998. "Sorption of Volatile Organic Chemicals in Plant Surfaces." *Environmental Science and Technology*, 32, pp. 1099-1104.

Wesely, M. L., P.V. Doskey, and J.D. Shannon, 2002. *Deposition Parameterizations for the Industrial Source Complex (ISC3) Model*. Environmental Research Division, Argonne National Laboratory, Argonne, IL. ANL/ER/TR-01/003. June 2002.