APPENDIX E

EXAMPLE CALCULATIONS
VINYL CHLORIDE, SUBSISTENCE FISHER LIFETIME (I) EXPOSURE SCENARIO

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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 at temperature
µg	microgram(s)
µg/m^3	microgram(s) per cubic meter
μ_w	viscosity of water at temperature
ρ_a	density of air
ρ_{soil}	solids particulate density
ρ_w	density of water
τ_{event}	lag time per event
a	empirical intercept coefficient
A_{beef}	concentration of chemical in beef tissue
ABS_d	dermal absorption fraction
A_{chick}	concentration of chemical in poultry meat
A_{egg}	concentration of chemical in poultry eggs
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
A_{milk}	concentration of chemical in dairy milk
A_{pork}	concentration of chemical in pork tissue
AT	averaging time
atm	atmosphere
A_w	water body surface area
b	empirical slope coefficient
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 poultry
Ba_{egg}	biotransfer factor for eggs
BAF_{fish}	bioaccumulation factor
Ba_{milk}	biotransfer factor for milk

Acronym/ Abbreviation	Definition
Ba_{pork}	biotransfer factor for pork
BCF_{fish}	bioconcentration factor
BD	soil bulk density
Br_{ag}	plant-to-soil bioconcentration factor for above-ground produce
Bs	soil bioavailability factor
Bv_{ag}	air-to-plant biotransfer factor
BW	body weight
C	USLE cover management factor
$C_{(air)}$	concentration of chemical in air
$C_{(air),acute}$	acute air concentration
$Cancer\ Risk_D$	excess lifetime cancer risk via inhalation
$Cancer\ Risk_I$	excess lifetime cancer risk from indirect exposures
$C_{aqueous}$	concentration of chemical in maternal breast milk aqueous phase
C_{BS}	bed sediment concentration
C_d	drag coefficient
C_{dw}	chemical concentration in the dissolved water phase
C_{fish}	chemical concentration in fish
cm	centimeter(s)
cm^2	square centimeter(s)
cm^3	cubic centimeter(s)
$C_{milkfat}$	concentration of chemical in maternal breast milk fat
COPC	chemical of potential concern
CR_{ag}	consumption rate of above-ground exposed fruits and vegetables
CR_{beef}	consumption rate of beef
CR_{bg}	consumption of below-ground vegetables
CR_{chick}	consumption rate of poultry
CR_{egg}	consumption rate of eggs
CR_{fish}	consumption rate of fish
CR_{milk}	consumption rate of dairy milk
CR_{pork}	consumption rate of pork
CR_{pp}	consumption rate of above-ground protected fruits and vegetables
CR_{soil}	consumption rate of soil
CR_{sw}	rate of consumption of surface water
Cs	chemical concentration in soil
CSF	cancer slope factor
CSF_I	inhalation cancer slope factor
CSF_O	oral cancer slope factor
Cs_{tD}	soil concentration at time tD

Acronym/ Abbreviation	Definition
C_{wctot}	total chemical concentration in water column
C_{wtot}	total water concentration, including water column and bed sediment
Cyv	vapor phase air concentration
Cywv	watershed vapor phase air concentration
D_a	diffusivity of chemical in air
DAD_{soil}	dermal absorbed dose from soil
DAD_{water}	dermal absorbed dose from water
DA_{event}	dermally absorbed dose per event
d_{bs}	depth of upper benthic layer
Ds	deposition term
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
Dytwp	yearly watershed total deposition from particle phase
Dytwv	yearly watershed total 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
Dywv	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
EC	inhalation exposure concentration
$EC_{VC,early\ life}$	additional early-life inhalation exposure concentration of vinyl chloride
ED	exposure duration
EDS	Explosive Destruction System
EF	exposure frequency
ER	soil enrichment ratio
ET	exposure time
E_v	average annual evapo-transpiration
EV	event frequency
F	fraction of plant grown on contaminated soil
FA	fraction absorbed water
F_{ag}	fraction of above-ground fruits and vegetables that are contaminated
F_{beef}	fraction of consumed beef that is contaminated
F_{bg}	fraction of below-ground vegetables that is contaminated

Acronym/ Abbreviation	Definition
f_{bs}	fraction of total water body chemical concentration that occurs in benthic sediment
F_{chick}	fraction of consumed poultry that is contaminated
F_{egg}	fraction of consumed eggs that are contaminated
F_{fish}	fraction of consumed fish that is contaminated
F_{milk}	fraction of consumed dairy milk that is contaminated
F_{pork}	fraction of consumed pork that is contaminated
F_{soil}	fraction of consumed soil that is contaminated
F_{sw}	swimming frequency
F_v	fraction of air concentration in vapor phase
Fw	fraction of wet deposition that adheres to plant
f_{wc}	fraction of total water body chemical concentration that occurs in the water column
g	gram
g/m^2-yr	gram per square meter-year
g/s	gram per second
H	Henry's Law constant
HI	hazard index
HQ	hazard quotient
HQ_D	hazard quotient for direct exposures
HQ_I	hazard quotient for indirect exposures
I	average annual irrigation
I_{ag}	daily intake of chemical from fruits and vegetables
I_{beef}	daily intake of chemical from beef
I_{bm}	daily intake of chemical from breast milk
I_{chick}	daily intake of chemical from poultry meat
I_{direct}	direct inhalation intake of chemical
I_{egg}	daily intake of chemical from eggs
I_{fish}	daily intake of chemical from fish
$I_{indirect}$	total indirect exposure
$I_{indirect(earlylife)}$	early-life indirect exposure to vinyl chloride
$I_{ingested}$	average daily ingestion dose
I_{milk}	daily intake of chemical from dairy milk
I_{pork}	daily intake of chemical from pork
IR	inhalation rate
I_{soil}	daily intake of chemical from soil
I_{sw}	daily intake of chemical from incidental ingestion of surface water
I_{total}	total daily intake of chemical through ingestion

Acronym/ Abbreviation	Definition
k	von Karman's constant
K	Kelvin
K	USLE erodibility factor
k_b	benthic burial rate constant
Kd_{bs}	bed sediment/sediment pore water partition coefficient
Kd_s	soil-water partition coefficient
Kd_{sw}	suspended sediment/surface water partition coefficient
kg	kilogram
K_G	gas phase transfer coefficient
K_L	liquid phase transfer coefficient
kp	plant surface loss coefficient
K_p	dermal permeability coefficient of chemical in water
ks	soil loss constant
kse	loss constant due to soil erosion
ksg	loss constant due to degradation
ksl	loss constant due to leaching
ksr	loss constant due to surface runoff
ksv	loss constant due to volatilization
k_v	water column volatilization rate constant
K_v	overall transfer rate
k_{wt}	total water body dissipation rate constant
ℓ	liter
L_{Dep}	direct deposition load to water body
L_{Dif}	vapor phase diffusion load to water body
L_E	soil erosion load to water body
L_R	pervious surface runoff load to water body
L_{RI}	impervious surface runoff load to water body
LS	USLE length-slope factor
L_T	total chemical load to water body
m^2	square meter
m^3	cubic meter
MF	metabolism factor
mg	milligram
mℓ	milliliter
mol	mole
P	average annual precipitation
PCAPP	Pueblo Chemical Agent-Destruction Pilot Plant
PCD	Pueblo Chemical Depot

Acronym/ Abbreviation	Definition
Pd	chemical concentration in plant due to direct deposition
PF	USLE supporting practice factor
Pr	chemical concentration in above-ground plants due to root uptake from soil
Pr_{bg}	chemical concentration in below-ground plants due to root uptake from soil
P_{total}	total concentration of chemical in plant
Pv	chemical concentration in the plant due to air-to-plant transfer
Q	stack emission rate
Qp	animal consumption rate of plant
Qs	animal consumption rate of soil
R	universal gas constant
RCF	root concentration factor
RF	USLE rainfall (or erosivity) factor
RfC	inhalation reference concentration
RfD	reference dose
RO	average annual runoff
Rp	interception fraction of edible portion of plant
s	second
SA	skin surface area available for contact
SD	watershed sediment delivery ratio
T_1	time at the beginning of emission
T_2	exposure duration
T_a	ambient air temperature
tD	total time period over which deposition occurs
t_{event}	duration of the swimming event
Tp	length of plant exposure to deposition of edible portion of plant, per harvest
TSS	total suspended solids
T_{wk}	water body temperature
USLE	Universal Soil Loss Equation
Vf_x	average volumetric flow rate through water body
VG_{ag}	above-ground fruit/vegetable correction factor
$VG_{rootveg}$	correction factor for below-ground produce
W	wind speed
X_e	unit soil loss
Yp	yield or standing crop biomass of the edible portion of the plant
yr	year

Acronym/ Abbreviation	Definition
Z_s	soil mixing depth

E EXAMPLE CALCULATIONS – VINYL CHLORIDE, SUBSISTENCE FISHER LIFETIME (I) EXPOSURE SCENARIO

E.1 OVERVIEW

This appendix contains calculations required to determine the carcinogenic risk and noncarcinogenic hazard to the subsistence fisher lifetime (I) exposure scenario (i.e., exposure to vinyl chloride for a subsistence fisher beginning at birth, continuing directly and indirectly for the 5-year operational period, and indirectly for the remaining 25 years of the exposure duration). The basis and all equations required to arrive at the risk and hazard estimates for exposure to vinyl chloride are included as presented in Appendix D. Equations presented herein are numbered as they appear in Appendix D.

For equations that include input parameters with differing values based on time period (infant, child, or adult) and/or type of effect (carcinogenic or noncarcinogenic), summary tables are provided below the calculations in this appendix to show the resulting values for each of the six time period/effect combinations. The equations shown with actual parameter values inserted always use the parameter values for the first value listed in the table. Because vinyl chloride is not considered to be found in breast milk, ingestion of breast milk for the infant portion of the exposure scenario is not covered in this appendix. Vinyl chloride is one of only three chemicals of potential concern (COPC) included in this MPHRA with early-life susceptibility data, and therefore early-life exposure for carcinogenic effects of vinyl chloride was included in this MPHRA and detailed in these example calculations in this appendix where appropriate.

This set of example calculations is included as a guide in the process of arriving at risk and hazard estimates. The final result of these calculations was summed with the corresponding results from all the other COPCs to arrive at final overall risk and hazard estimates for potential exposure to COPCs emitted from the Pueblo Chemical Agent-Destruction Pilot Plant (PCAPP) and Explosive Destruction System (EDS) to be operated at the Pueblo Chemical Depot (PCD). Minor differences between results reported herein and those obtained directly from the post-processor are due to rounding in the post-processor.

E.2 AIR CONCENTRATION

The American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD) air dispersion model was used to calculate air concentrations as well as both wet and dry deposition rates. The air parameters were calculated at two different locations: 1) the receptors of maximum impact and 2) the receptor over a body of water with maximum impact. The AERMOD post-processor was used to adjust the unit response vinyl chloride air parameters by the actual vinyl chloride emission rates from PCAPP and EDS sources. The adjusted outputs are reported in Table E-1. Adjusted air parameters are used throughout this appendix with an emission rate of 1 gram per second (g/s) (since the air parameters have already been adjusted). The units of the adjusted outputs are micrograms per cubic meter ($\mu g/m^3$) and grams per square meter-year (g/m^2-yr) rather than microgram per cubic meter per gram per second ($\mu g/m^3$ per g/s) and gram per square meter-year per gram per second (g/m^2-yr per g/s) due to the adjustment. In the calculations, units without the adjustment are shown so that inclusion of an emission rate in g/s results in correct units for calculated values.

Table E-1. AERMOD Outputs for Vinyl Chloride

Parameter	Symbol	Value	Units
Overall – adjusted vapor phase air concentration	Cyv	1.52×10^{-3}	μg/m^3
Overall – adjusted particle phase air concentration	Cyp	1.50×10^{-3}	μg/m^3
Overall – adjusted dry deposition from vapor phase	Dydv	4.14×10^{-4}	g/m^2-yr
Overall – adjusted wet deposition from vapor phase	Dywv	1.31×10^{-5}	g/m^2-yr
Overall – adjusted dry deposition from particle phase	Dydp	2.12×10^{-4}	g/m^2-yr
Overall – adjusted wet deposition from particle phase	Dywp	0	g/m^2-yr
Watershed – adjusted vapor phase air concentration	Cywv	4.23×10^{-4}	μg/m^3
Watershed – adjusted particle phase air concentration	Cywp	4.08×10^{-4}	μg/m^3
Watershed – adjusted dry deposition from vapor phase	Dywdv	8.93×10^{-5}	g/m^2-yr
Watershed – adjusted wet deposition from vapor phase	Dywwv	5.40×10^{-6}	g/m^2-yr
Watershed – adjusted dry deposition from particle phase	Dywdp	6.75×10^{-5}	g/m^2-yr
Watershed – adjusted wet deposition from particle phase	Dywwp	0	g/m^2-yr

E.3 SOIL CONCENTRATION

The concentration of vinyl chloride in soil was calculated using the equations presented in Appendix D. This section walks through the calculations necessary to arrive at the final soil concentrations of vinyl chloride, for carcinogenic and noncarcinogenic effects for all age group portions in the subsistence fisher lifetime (I) exposure scenario, starting with soil losses due to various processes and working up to the concentration of vinyl chloride in soil. Soil loss equations are presented first because they are used in the calculation of the total concentration in soil.

The soil loss constant due to leaching was calculated using Equation D-3. If the sum of precipitation and irrigation was less than the sum of runoff and evaporation (i.e. the numerator of Equation D-3 was negative), then *ksl* was set to zero.

$$ksl = \frac{P + I - RO - E_V}{\theta_{sw} \cdot Z_s \cdot [1.0 + (BD \cdot Kd_s / \theta_{sw})]} \qquad \text{Eq. D-3}$$

where

ksl	=	loss constant due to leaching (yr^{-1})
P	=	average annual precipitation (31.5 cm/yr)
I	=	average annual irrigation (0 cm/yr)
RO	=	average annual runoff (1.27 cm/yr)
E_v	=	average annual evapo-transpiration (121.9 cm/yr)
θ_{SW}	=	soil volumetric water content (0.2 mℓ/cm^3)
Z_s	=	soil mixing depth (2 cm)
Kd_s	=	soil-water partition coefficient (0.037 cm^3/g)
BD	=	soil bulk density (1.5 g/cm^3)

$$ksl = \frac{31.5 + 0 - 1.27 - 121.9}{0.2 \cdot 2 \cdot [1 + (1.5 \cdot 0.037 / 0.2)]} = -179 \therefore ksl = 0 \ yr^{-1}$$

The soil loss constant due to runoff was calculated using Equation D-4.

$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \frac{1}{1.0 + (Kd_s \cdot BD / \theta_{sw})} \qquad \text{Eq. D-4}$$

where

ksr	=	loss constant due to surface runoff (yr^{-1})
RO	=	average annual runoff (1.27 cm/yr)
θ_{SW}	=	soil volumetric water content (0.2 mℓ/cm^3)
Z_s	=	soil mixing depth (2 cm)
Kd_s	=	soil-water partition coefficient (0.037 cm^3/g)
BD	=	soil bulk density (1.5 g/cm^3)

$$ksr = \frac{1.27}{0.2 \cdot 2} \cdot \frac{1}{1 + (0.037 \cdot 1.5 / 0.2)} = 2.49\ yr^{-1}$$

The soil loss constant due to volatilization was calculated using Equation D-5.

$$ksv = \left(\frac{3.1536 \cdot 10^7 \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \frac{D_a}{Z_s} \cdot \left[1 - \frac{BD}{\rho_{soil}} - \theta_{sw} \right] \qquad \text{Eq. D-5}$$

where

ksv	=	loss constant due to volatilization (yr^{-1})
3.1536×10^7	=	unit conversion (s/yr)
H	=	Henry's Law constant (0.027 atm-m^3/mol)
Z_s	=	soil mixing depth (2 cm)
Kd_s	=	soil-water partition coefficient (0.037 cm^3/g)
R	=	universal gas constant (8.205 x 10^{-5} atm-m^3/mol-K)
BD	=	soil bulk density (1.5 g/cm^3)
T_a	=	ambient air temperature (298 K)
ρ_{soil}	=	solids particulate density (2.7 g/cm^3)
D_a	=	diffusivity of vinyl chloride in air (0.106 cm^2/sec)
θ_{SW}	=	soil volumetric water content (0.2 mℓ/cm^3 soil)

$$ksv = \left(\frac{3.1536 \cdot 10^7 \cdot 0.027}{2 \cdot 0.037 \cdot 8.205 \cdot 10^{-5} \cdot 298 \cdot 1.5} \right) \cdot \frac{0.106}{2} \cdot \left[1 - \frac{1.5}{2.7} - 0.2 \right] = 4{,}064{,}513.63\ yr^{-1}$$

The soil loss constant due to erosion (*kse*) was set to the default value of zero for vinyl chloride.

The soil loss constant due to degradation (*ksg*) is a chemical-specific value (1.41 yr^{-1} for vinyl chloride). Section F.4.1 of Appendix F describes the methods used to obtain the chemical-specific values for this parameter.

The overall soil loss constant was calculated as the sum of soil loss constants due to individual processes using Equation D-2.

$$ks = ksl + kse + ksr + ksg + ksv \qquad \text{Eq. D-2}$$

where

ks	=	soil loss constant (yr^{-1})
ksl	=	loss constant due to leaching (0 yr^{-1})
kse	=	loss constant due to soil erosion (0 yr^{-1})
ksr	=	loss constant due to surface runoff (2.49 yr^{-1})
ksg	=	loss constant due to degradation (1.41 yr^{-1})
ksv	=	loss constant due to volatilization (4,064,513.63 yr^{-1})

$$ks = 0 + 0 + 2.49 + 1.41 + 4{,}064{,}513.63 = 4{,}064{,}517.52 \ \ yr^{-1}$$

Deposition of vinyl chloride onto soil was calculated using Equation D-1. Model outputs were adjusted with vinyl chloride emission rates using a post-processor. As a result, an emission rate of 1 g/s is used throughout these calculations so as not to adjust the outputs twice.

$$Ds = \frac{100 \cdot Q}{Z_s \cdot BD} \cdot [F_v\,(Dydv + Dywv) + (Dydp + Dywp) \cdot (1 - F_v)] \qquad \text{Eq. D-1}$$

where

Ds	=	deposition term (mg/kg-yr)
Dydp	=	adjusted dry deposition from particle phase (2.12 x 10^{-4} s/m^2-yr)
Dywp	=	adjusted wet deposition from particle phase (0 s/m^2-yr)
Dydv	=	adjusted dry deposition from vapor phase (4.14 x 10^{-4} s/m^2-yr)
Dywv	=	adjusted wet deposition from vapor phase (1.31 x 10^{-5} s/m^2-yr)
100	=	unit conversion factor ([mg-m^2]/[kg-cm^2])
Z_s	=	soil mixing depth (2 cm)
BD	=	soil bulk density (1.5 g/cm^3)
Q	=	stack emission rate (1 g/s)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)

$$Ds = \frac{100 \cdot 1}{2 \cdot 1.5} \cdot \left[1 \cdot \left(4.14 \cdot 10^{-4} + 1.31 \cdot 10^{-5}\right) + \left(0 + 2.12 \cdot 10^{-4}\right) \cdot \left(1 - 1\right)\right] = 1.42 \cdot 10^{-2} \ \frac{mg}{kg \cdot yr}$$

Equation D-7 was used to calculate vinyl chloride soil concentrations for noncarcinogenic effects and represents the highest annual average vinyl chloride concentration.

$$Cs_{tD} = \frac{Ds \cdot [1 - exp(-ks \cdot tD)]}{ks} \qquad \text{Eq. D-7}$$

where

Cs_{tD}	=	soil concentration at time tD (mg/kg)
Ds	=	deposition term (1.42 x 10^{-2} mg/kg-yr)
ks	=	soil loss constant (4,064,517.52 yr^{-1})
tD	=	total time period over which deposition occurs (5 yr)

$$Cs_{tD} = \frac{1.42 \cdot 10^{-2} \cdot [1 - exp(-4064517.52 \cdot 5)]}{4064517.52} = 3.49 \cdot 10^{-9}\ \frac{mg}{kg}$$

Equation D-6a was used to calculate vinyl chloride soil concentrations for carcinogenic effects for the adult portion of the exposure scenario and represents the soil concentration averaged over the exposure duration. The concentration is averaged over the entire 30 year exposure duration rather than just the 24 years of exposure as an adult.

$$Cs = \frac{\frac{Ds \cdot tD - Cs_{tD}}{ks} + \frac{Cs_{tD}}{ks} \cdot [1.0 - exp(-ks \cdot (T_2 - tD))]}{(T_2 - T_1)} \qquad \text{Eq. D-6a}$$

where

Cs	=	vinyl chloride concentration in soil (mg/kg)
Ds	=	deposition term (1.42 x 10^{-2} mg/kg-yr)
ks	=	soil loss constant (4,064,517.52 yr^{-1})
tD	=	total time period over which deposition occurs (5 yr)
Cs_{tD}	=	soil concentration at time tD (3.49 x 10^{-9} mg/kg)
T_2	=	exposure duration (30 yr)
T_1	=	time at the beginning of emission (0 yr)

$$Cs = \frac{\frac{1.42 \cdot 10^{-2} \cdot 5 - 3.49 \cdot 10^{-9}}{4064517.52} + \frac{3.49 \cdot 10^{-9}}{4064517.52} \cdot [1.0 - exp(-4064517.52 \cdot (30 - 5))]}{(30 - 0)} = 5.82 \cdot 10^{-10}\ \frac{mg}{kg}$$

Equation D-6b was used to calculate vinyl chloride soil concentrations for carcinogenic effects for the infant and child portions of the exposure scenario and represents the soil concentration averaged over the 5-year operational period of the PCAPP operation.

$$Cs = \frac{Ds}{ks \cdot (tD - T_1)} \cdot \left(\left[tD + \frac{exp(-ks \cdot tD)}{ks} \right] - \left[T_1 + \frac{exp(-ks \cdot T_1)}{ks} \right] \right) \qquad \text{Eq. D-6b}$$

where

Cs	=	chemical concentration in soil (mg/kg)
Ds	=	deposition term (1.42 x 10^{-2} mg/kg-yr)

ks	=	soil loss constant (4,064,517.52 yr^{-1})
tD	=	total time period over which deposition occurs (5 yr)
T_1	=	time at the beginning of emission (0 yr)

$$Cs = \frac{1.42 \cdot 10^{-2}}{4064517.52 \cdot (5-0)} \cdot \left(\left[5 + \frac{exp(-4064517.52 \cdot 5)}{4064517.52} \right] - \left[0 + \frac{exp(-4064517.52 \cdot 0)}{4064517.52} \right] \right) = 3.49 \cdot 10^{-9} \frac{mg}{kg}$$

Time Period	Effect	Soil Concentration (C_S) (mg/kg)
Adult	Carcinogenic	5.82×10^{-10}
Adult	Noncarcinogenic	3.49×10^{-9}
Child	Carcinogenic	3.49×10^{-9}
Child	Noncarcinogenic	3.49×10^{-9}
Infant	Carcinogenic	3.49×10^{-9}
Infant	Noncarcinogenic	3.49×10^{-9}

E.4 SURFACE WATER CONCENTRATION

Surface water concentrations of vinyl chloride due to direct deposition, runoff, erosion, and diffusion were calculated for the water body in the area with the maximum modeled air concentration and deposition rates. Wet and dry deposition rates were determined through air dispersion modeling. Calculations are presented in this section starting with calculation of parameters used to calculate individual loads and working up to the total dissolved water concentration of vinyl chloride.

In order to calculate the load to a water body due to diffusion, liquid, gas, and overall mass transfer coefficients must be calculated. The liquid phase mass transfer coefficient was calculated using equation D-17.

$$K_L = C_d^{0.5} \cdot W \cdot \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_w}{\rho_w \cdot D_w} \right)^{-0.67} \cdot 3.1536 \cdot 10^7 \qquad \text{Eq. D-17}$$

where

K_L	=	liquid phase transfer coefficient (m/yr)
D_w	=	diffusivity of vinyl chloride in water (1.23 x 10^{-5} cm^2/s)
W	=	wind speed (3.9 m/s)
C_d	=	drag coefficient (0.0011 dimensionless)
ρ_a	=	density of air (0.0012 g/cm^3)
ρ_w	=	density of water (1 g/cm^3)
k	=	von Karman's constant (0.4 dimensionless)
λ_z	=	dimensionless viscous sublayer thickness (4 dimensionless)
μ_w	=	viscosity of water at temperature (0.0169 g/cm-s)
3.1536×10^7	=	units conversion factor (s/yr)

$$K_L = 0.0011^{0.5} \cdot 3.9 \cdot \left(\frac{0.0012}{1} \right)^{0.5} \cdot \frac{0.4^{0.33}}{4} \cdot \left(\frac{0.0169}{1 \cdot 1.23 \cdot 10^{-5}} \right)^{-0.67} \cdot 3.1536 \cdot 10^7 = 206.22 \frac{m}{yr}$$

The gas phase mass transfer coefficient was calculated using Equation D-18.

$$K_G = C_d^{0.5} \cdot W \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a} \right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Eq. D-18}$$

where

K_G	=	gas phase transfer coefficient (m/yr)
D_a	=	diffusivity of vinyl chloride in air (0.106 cm^2/s)
W	=	wind speed (3.9 m/s)
C_d	=	drag coefficient (0.0011 dimensionless)
ρ_a	=	density of air (0.0012 g/cm^3)
k	=	von Karman's constant (0.4 dimensionless)
λ_z	=	dimensionless viscous sublayer thickness (4 dimensionless)
μ_a	=	viscosity of air at temperature (1.81 x 10^{-4} g/cm-s)
3.1536×10^7	=	units conversion factor (s/yr)

$$K_G = 0.0011^{0.5} \cdot 3.9 \cdot \frac{0.4^{0.33}}{4} \cdot \left(\frac{1.81 \cdot 10^{-4}}{0.0012 \cdot 0.106} \right)^{-0.67} \cdot 3.1536 \times 10^7 = 595{,}044 \frac{m}{yr}$$

The overall mass transfer rate was calculated using Equation D-16.

$$K_v = \left[K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right]^{-1} \cdot \theta^{(T_{wk} - 293)} \qquad \text{Eq. D-16}$$

where

K_v	=	overall transfer rate (m/yr)
K_L	=	liquid phase transfer coefficient (206.22 m/yr)
K_G	=	gas phase transfer coefficient (595,044 m/yr)
H	=	Henry's Law constant (0.027atm-m^3/mol)
R	=	universal gas constant (8.205 x 10^{-5} atm-m^3/mol-K)
T_{wk}	=	water body temperature (298 K)
θ	=	temperature correction factor (1.026 dimensionless)

$$K_v = \left[206.22^{-1} + \left(595044 \cdot \frac{0.027}{8.205 \cdot 10^{-5} \cdot 298} \right)^{-1} \right]^{-1} \cdot 1.026^{(298-293)} = 234.39 \frac{m}{yr}$$

The vapor phase chemical diffusion load of vinyl chloride to the water body was calculated using Equation D-15.

$$L_{Dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cyw \cdot A_w \cdot 10^{-6}}{\frac{H}{R \cdot T_{wk}}} \qquad \text{Eq. D-15}$$

where

L_{Dif}	=	vapor phase diffusion load to water body (g/yr)
Q	=	vinyl chloride stack emission rate (1 g/s)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
K_v	=	overall transfer rate (234.39 m/yr)
$Cywv$	=	adjusted watershed vapor phase air concentration (4.23×10^{4} µg/m^3 per g/s)
A_w	=	water body surface area (75,000 m^2)
H	=	Henry's Law constant (0.027 atm-m^3/mol)
R	=	universal gas constant (8.205×10^{-5} atm-m^3/mol-K)
T_{wk}	=	water body temperature (298 K)
10^{-6}	=	units conversion factor (g/µg)

$$L_{Dif} = \frac{234.39 \cdot 1 \cdot 1 \cdot 4.23 \cdot 10^{-4} \cdot 75{,}000 \cdot 10^{-6}}{\dfrac{0.027}{8.205 \cdot 10^{-5} \cdot 298}} = 6.73 \cdot 10^{-3}$$

The unit soil loss was calculated using Equation D-13.

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \qquad \text{Eq. D-13}$$

where

X_e	=	unit soil loss (kg/m^2-yr)
RF	=	USLE rainfall (or erosivity) factor (31 yr^{-1})
K	=	USLE erodibility factor (0.37 ton/acre)
LS	=	USLE length-slope factor (1.5 dimensionless)
C	=	USLE cover management factor (0.1 dimensionless)
PF	=	USLE supporting practice factor (1 dimensionless)
907.18	=	conversion factor (kg/ton)
4047	=	conversion factor (m^2/acre)

$$X_e = 31 \cdot 0.37 \cdot 1.5 \cdot 0.1 \cdot 1 \cdot \frac{907.18}{4047} = 0.39 \frac{kg}{m^2 \cdot yr}$$

The sediment delivery ratio was calculated using Equation D-14.

$$SD = a \cdot (A_L)^{-b} \qquad \text{Eq. D-14}$$

where

SD	=	watershed sediment delivery ratio (dimensionless)
A_L	=	total watershed area receiving chemical deposition (183,516,000 m^2)
b	=	empirical slope coefficient (0.125 dimensionless)
a	=	empirical intercept coefficient (1.9 dimensionless)

$$SD = 1.9 \cdot (183{,}516{,}000)^{-0.125} = 0.176$$

The soil erosion load of vinyl chloride to the water body was calculated using Equation D-12.

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001 \qquad \text{Eq. D-12}$$

where

L_E	=	soil erosion load to water body (g/yr)
X_e	=	unit soil loss (0.39 kg/m^2-yr)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
BD	=	soil bulk density (1.5 g/cm^3)
θ_{SW}	=	soil volumetric water content (0.2 cm^3/cm^3)
Kd_s	=	soil-water partition coefficient (0.037 ℓ/kg)
A_L	=	total watershed area receiving vinyl chloride deposition (183,516,000 m^2)
A_I	=	impervious watershed area receiving vinyl chloride deposition (3,670,320 m^2)
SD	=	watershed sediment delivery ratio (0.176 dimensionless)
ER	=	soil enrichment ratio (3 dimensionless)
0.001	=	units conversion factor [g/kg]/[mg/kg])

$$L_E = 0.39 \cdot (183{,}516{,}000 - 3{,}670{,}320) \cdot 0.176 \cdot 3 \cdot \frac{5.82 \cdot 10^{-10} \cdot 0.037 \cdot 1.5}{0.2 + 0.037 \cdot 1.5} \cdot 0.001 = 4.68 \cdot 10^{-6}\ \frac{g}{yr}$$

Time Period	Effect	Soil Erosion Load (L_E) (g/yr)
Adult	Carcinogenic	4.68 x 10^{-6}
Adult	Noncarcinogenic	2.81 x 10^{-5}
Child	Carcinogenic	2.81 x 10^{-5}
Child	Noncarcinogenic	2.81 x 10^{-5}
Infant	Carcinogenic	2.81 x 10^{-5}
Infant	Noncarcinogenic	2.81 x 10^{-5}

The pervious surface runoff load was calculated using Equation D-11.

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01 \qquad \text{Eq. D-11}$$

where

L_R	=	pervious surface runoff load to water body (g/yr)
RO	=	average annual runoff (1.27 cm/yr)

Cs	=	vinyl chloride concentration in soil (5.82×10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49×10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
BD	=	soil bulk density (1.5 g/cm^3)
Kd_s	=	soil-water partition coefficient (0.037 cm^3/g)
A_L	=	total watershed area receiving vinyl chloride deposition (183,516,000 m^2)
A_I	=	impervious watershed area receiving vinyl chloride deposition (3,670,320 m^2)
0.01	=	units conversion factor (kg-cm^2/mg-m^2)
θ_{SW}	=	soil volumetric water content (0.2 cm^3/cm^3)

$$L_R = 1.27 \cdot (183{,}516{,}000 - 3{,}670{,}320) \cdot \frac{5.82 \cdot 10^{-10} \cdot 1.5}{0.2 + 0.037 \cdot 1.5} \cdot 0.01 = 7.80 \cdot 10^{-3}\ \frac{g}{yr}$$

Time Period	**Effect**	**Pervious Surface Runoff Load (L_R) (g/yr)**
Adult	Carcinogenic	7.80×10^{-3}
Adult	Noncarcinogenic	4.68×10^{-2}
Child	Carcinogenic	4.68×10^{-2}
Child	Noncarcinogenic	4.68×10^{-2}
Infant	Carcinogenic	4.68×10^{-2}
Infant	Noncarcinogenic	4.68×10^{-2}

The impervious surface runoff load was calculated using Equation D-10.

$$L_{RI} = Q \cdot \left[F_v \cdot Dytwv + (1 - F_v) \cdot Dytwp\right] \cdot A_I \qquad \text{Eq. D-10}$$

where

L_{RI}	=	impervious surface runoff load to water body (g/yr)
Q	=	vinyl chloride stack emission rate (1 g/s)
F_v	=	fraction of vinyl chloride in vapor phase (1 dimensionless)
Dytwv	=	adjusted watershed total deposition from vapor phase (*Dywwv* + *Dydv*) (9.47×10^{-5} g/m^2-yr per g/s)
Dytwp	=	adjusted watershed total deposition from particle phase (Dywdp + Dywwp) (6.75×10^{-5} g/m^2-yr per g/s)
A_I	=	impervious watershed area receiving vinyl chloride deposition (3,670,320 m^2)

$$L_{RI} = 1 \cdot \left[1 \cdot 9.47 \cdot 10^{-5} + (1-1) \cdot 6.75 \cdot 10^{-5}\right] \cdot 3{,}670{,}320 = 3.48 \cdot 10^{2}\ \frac{g}{yr}$$

The vinyl chloride load to the water body due to direct deposition was calculated using Equation D-9.

$$L_{Dep} = Q \cdot \left[F_v \cdot Dytwv + (1 - F_v) \cdot Dytwp\right] \cdot A_w \qquad \text{Eq. D-9}$$

where

L_{Dep}	=	direct deposition load to water body (g/yr)
Q	=	vinyl chloride stack emission rate (1 g/s)
F_v	=	fraction of vinyl chloride in vapor phase (1 dimensionless)
Dytwv	=	adjusted watershed total deposition from vapor phase (*Dywwv* + *Dydv*) (9.47 x 10^{-5} g/m^2-yr per g/s)
Dytwp	=	adjusted watershed total deposition from particle phase (*Dywdp* + *Dywwp*) (6.75 x 10^{-5} g/m^2-yr per g/s)
A_w	=	water body area (75,000 m^2)

$$L_{Dep} = 1 \cdot \left[1 \cdot 9.47 \cdot 10^{-5} + (1-1) \cdot 6.75 \cdot 10^{-5}\right] \cdot 75{,}000 = 7.10 \frac{g}{yr}$$

The total vinyl chloride load to the water body was calculated as the sum of the individual loads using Equation D-8.

$$L_T = L_{Dep} + L_{Dif} + L_{RI} + L_R + L_E \qquad \text{Eq. D-8}$$

where

L_T	=	total vinyl chloride load to water body (g/yr)
L_{Dep}	=	direct deposition load to water body (7.1 g/yr)
L_{Dif}	=	vapor phase diffusion load to water body (6.73 x 10^{-3} g/yr)
L_{RI}	=	impervious surface runoff load to water body (3.48 x 10^{2} g/yr)
L_R	=	pervious surface runoff load to water body (7.80 x 10^{-3} g/yr [carcinogenic effects, adult portion], 4.68 x 10^{-2} g/yr [carcinogenic effects, infant and child portions; noncarcinogenic effects])
L_E	=	soil erosion load to water body (4.68 x 10^{-6} g/yr [carcinogenic effects, adult portion], 2.81 x 10^{-5} g/yr [carcinogenic effects, infant and child portions; noncarcinogenic effects])

$$L_T = 7.10 + 6.73 \cdot 10^{-3} + 3.48 \cdot 10^{2} + 7.80 \cdot 10^{-3} + 4.68 \cdot 10^{-6} = 3.55 \cdot 10^{2} \frac{g}{yr}$$

Time Period	Effect	Total Load to Waterbody (L_T) (g/yr)
Adult	Carcinogenic	3.55 x 10^2
Adult	Noncarcinogenic	3.55 x 10^2
Child	Carcinogenic	3.55 x 10^2
Child	Noncarcinogenic	3.55 x 10^2
Infant	Carcinogenic	3.55 x 10^2
Infant	Noncarcinogenic	3.55 x 10^2

The fraction of the total water body vinyl chloride concentration that occurs in the water column was calculated using Equation D-20.

$$f_{wc} = \frac{\left(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}\right) \cdot \left(d_{wc}/d_z\right)}{\left(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}\right) \cdot \left(d_{wc}/d_z\right) + \left(\theta_{bs} + Kd_{bs} \cdot C_{BS}\right) \cdot \left(d_{bs}/d_z\right)} \qquad \text{Eq. D-20}$$

where

f_{wc} = fraction of total water body vinyl chloride concentration that occurs in the water column (dimensionless)
Kd_{sw} = suspended sediment/surface water partition coefficient (1.15 ℓ/kg)
TSS = total suspended solids (10 mg/ℓ)
10^{-6} = conversion factor (kg/mg)
d_{wc} = depth of water column (5 m)
d_{bs} = depth of upper benthic layer (0.03 m)
d_z = total water body depth (5.03 m), (d_{wc} + d_{bs})
θ_{bs} = bed sediment porosity (0.6 $ℓ_{water}$/ℓ)
Kd_{bs} = bed sediment/sediment pore water partition coefficient (0.62 ℓ/kg)
C_{BS} = bed sediment concentration (1.0 g/cm^3)

$$f_{wc} = \frac{\left(1 + 1.15 \cdot 10 \cdot 10^{-6}\right) \cdot (5.00/5.03)}{\left(1 + 1.15 \cdot 10 \cdot 10^{-6}\right) \cdot (5.00/5.03) + (0.6 + 0.62 \cdot 1) \cdot (0.03/5.03)} = 0.993$$

The fraction of the total water body vinyl chloride concentration that occurs in benthic sediments was calculated using Equation D-21.

$$f_{bs} = 1 - f_{wc} \qquad \text{Eq. D-21}$$

where

f_{bs} = fraction of total water body vinyl chloride concentration that occurs in benthic sediment (dimensionless)
f_{wc} = fraction of total water body vinyl chloride concentration that occurs in the water column (0.993 dimensionless)

$$f_{bs} = 1 - 0.993 = 7.27 \times 10^{-3}$$

The water column volatilization rate constant was calculated using Equation D-23.

$$k_v = \frac{K_V}{d_z \cdot \left(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}\right)} \qquad \text{Eq. D-23}$$

where

k_v	=	water column volatilization rate constant (yr^{-1})
K_v	=	overall transfer rate (234.39 m/yr)
d_z	=	total water body depth (5.03 m)
Kd_{sw}	=	suspended sediment/surface water partition coefficient (1.15 ℓ/kg)
TSS	=	total suspended solids (10 mg/ℓ)
10^{-6}	=	conversion factor (kg/mg)

$$k_v = \frac{234.39}{5.03 \cdot \left(1 + 1.15 \cdot 10 \cdot 10^{-6}\right)} = 46.60\ yr^{-1}$$

The benthic burial rate was calculated using Equation D-24.

$$k_b = \frac{X_e \cdot A_L \cdot SD \cdot 10^3 - Vf_x \cdot TSS}{A_w \cdot TSS} \cdot \frac{TSS \cdot 10^{-6}}{C_{BS} \cdot d_{bs}} \qquad \text{Eq. D-24}$$

where

k_b	=	benthic burial rate constant (yr^{-1})
X_e	=	unit soil loss (0.39 kg/m^2-yr)
A_L	=	total watershed area receiving vinyl chloride deposition (183,516,000 m^2)
SD	=	watershed sediment delivery ratio (0.176 dimensionless)
10^3	=	conversion factor (g/kg)
Vf_x	=	average volumetric flow rate through water body (2,680,560 m^3/yr)
TSS	=	total suspended solids (10 mg/ℓ)
A_w	=	water body surface area (75,000 m^2)
C_{BS}	=	bed sediment concentration (1 kg/ℓ)
d_{bs}	=	depth of upper benthic layer (0.03 m)
10^{-6}	=	conversion factor (kg/mg)

$$k_b = \frac{0.39 \cdot 183{,}516{,}000 \cdot 0.176 \cdot 10^3 - 2680560 \cdot 10}{75{,}000 \cdot 10} \cdot \frac{10 \cdot 10^{-6}}{1 \cdot 0.03} = 5.59\ yr^{-1}$$

The overall dissipation rate of vinyl chloride was calculated using Equation D-22.

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \qquad \text{Eq. D-22}$$

where

k_{wt}	=	total water body dissipation rate constant (yr^{-1})
f_{wc}	=	fraction of total water body vinyl chloride concentration that occurs in the water column (0.993 dimensionless)
k_v	=	water column volatilization rate constant (46.60 yr^{-1})

f_{bs}	=	fraction of total water body vinyl chloride concentration that occurs in benthic sediment (7.27 x 10^{-3} dimensionless)
k_b	=	benthic burial rate (5.59 yr^{-1})

$$k_{wt} = 0.993 \cdot 46.60 + 7.27 \text{ x } 10^{-3} \cdot 5.59 = 46.3\ yr^{-1}$$

The total water body concentration of vinyl chloride was calculated using Equation D-19.

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} \cdot + k_{wt} \cdot A_w \cdot (d_{wc} + d_{bs})} \qquad \text{Eq. D-19}$$

where

C_{wtot}	=	total water concentration, including water column and bed sediment (g/m^3)
L_T	=	total vinyl chloride load to water body (3.55 x 10^2 g/yr)
Vf_x	=	average volumetric flow rate through water body (2,680,560 m^3/yr)
f_{wc}	=	fraction of total water body vinyl chloride concentration that occurs in the water column (0.993 dimensionless)
k_{wt}	=	total water body dissipation rate constant (46.3 yr^{-1})
A_w	=	water body surface area (75,000 m^2)
d_{wc}	=	depth of water column (5 m)
d_{bs}	=	depth of upper benthic layer (0.03 m)

$$C_{wtot} = \frac{3.55 \cdot 10^2}{2680560 \cdot 0.993 \cdot + 46.3 \cdot 75{,}000 \cdot (5.00 + 0.03)} = 1.76 \cdot 10^{-5}\ \frac{g}{m^3}$$

The total water column concentration of vinyl chloride was calculated using Equation D-25.

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}} \qquad \text{Eq. D-25}$$

where

C_{wctot}	=	total vinyl chloride concentration in water column (mg/ℓ)
f_{wc}	=	fraction of total water body vinyl chloride concentration that occurs in the water column (0.993 dimensionless)
C_{wtot}	=	total water concentration, including water column and bed sediment (1.76 x 10^{-5} g/m^3)
d_{bs}	=	depth of upper benthic layer (0.03 m)
d_{wc}	=	depth of water column (5 m)

$$C_{wctot} = 0.993 \cdot 1.76 \cdot 10^{-5} \cdot \frac{5.00 + 0.03}{5.00} = 1.76 \cdot 10^{-5}\ \frac{g}{m^3}$$

The concentration of vinyl chloride dissolved in the water column was calculated using Equation D-26.

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 10^{-6}} \qquad \text{Eq. D-26}$$

where

C_{dw}	=	concentration of vinyl chloride in the dissolved water phase (mg/ℓ)
C_{wctot}	=	total vinyl chloride concentration in water column (1.76 x 10^{-5} mg/ℓ)
Kd_{sw}	=	suspended sediment/surface water partition coefficient (1.15 ℓ/kg)
TSS	=	total suspended solids (10 mg/ℓ)
10^{-6}	=	conversion factor (kg/mg)

$$C_{dw} = \frac{1.76 \cdot 10^{-5}}{1 + 1.15 \cdot 10 \cdot 10^{-6}} = 1.76 \cdot 10^{-5} \frac{mg}{\ell}$$

E.5 FRUIT AND VEGETABLE CONCENTRATION

Direct deposition, air to plant transfer, and root uptake of vinyl chloride all contribute to the total vinyl chloride concentration in fruits and vegetables. The vinyl chloride concentration in fruits and vegetables due to direct deposition was calculated using Equation D-27.

$$Pd = \frac{1000 \cdot Q \cdot (1.0 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - exp(-kp \cdot Tp)]}{Yp \cdot kp} \qquad \text{Eq. D-27}$$

where

Pd	=	vinyl chloride concentration in plant due to direct deposition (mg/kg)
1000	=	unit conversion factor (mg/g)
Q	=	vinyl chloride stack emission rate (1 g/s)
Dydp	=	adjusted dry deposition from particle phase (2.12 x 10^{-4} s/m^2-yr)
Fw	=	fraction of wet deposition that adheres to plant (0.6 dimensionless)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
Dywp	=	adjusted wet deposition from particle phase (0 s/m^2-yr)
Rp	=	interception fraction of edible portion of plant (0.39 dimensionless)
kp	=	plant surface loss coefficient (18 yr^{-1})
Tp	=	length of plant exposure to deposition of edible portion of plant, per harvest (0.16 yr)
Yp	=	yield or standing crop biomass of the edible portion of the plant (2.24 kg/m^2)

$$Pd = \frac{1000 \cdot 1 \cdot (1.0 - 1) \cdot [2.12 \cdot 10^{-4} + (0.6 \cdot 0)] \cdot 0.39 \cdot [1.0 - exp(-18 \cdot 0.16)]}{2.24 \cdot 18} = 0 \frac{mg}{kg}$$

The vinyl chloride concentration in plants due to air to plant transfer was calculated using Equation D-28.

$$Pv = Q \cdot F_V \cdot \frac{Cyv \cdot Bv_{ag} \cdot VG_{ag}}{\rho_a} \qquad \text{Eq. D-28}$$

where

Pv	=	vinyl chloride concentration in the plant due to air-to-plant transfer (mg/kg)
Q	=	vinyl chloride stack emission rate (1 g/s)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
Cyv	=	adjusted vapor phase air concentration (1.52 x 10^{-3} μg/m^3 per g/s)
VG_{ag}	=	above-ground fruit/vegetable correction factor (1 dimensionless)
Bv_{ag}	=	air-to-plant biotransfer factor (6.41 x 10^{-5} [mg pollutant/g plant tissue]/[mg vinyl chloride/g air])
ρ_a	=	density of air (1,200 g/m^3)

$$Pv = 1 \cdot 1 \cdot \frac{1.52 \cdot 10^{-3} \cdot 6.41 \cdot 10^{-5} \cdot 1}{1200} = 8.12 \cdot 10^{-11}\ \frac{mg}{kg}$$

The vinyl chloride concentration in above ground fruits and vegetables due to root uptake was calculated using Equation D-29.

$$Pr = Cs \cdot Br_{ag} \qquad \text{Eq. D-29}$$

where

Pr	=	vinyl chloride concentration in plant due to root uptake from soil (mg/kg)
Cs	=	vinyl chloride concentration in soil (5.82 X 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 X 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Br_{ag}	=	plant-to-soil bioconcentration factor for above ground produce (6.01 dimensionless)

$$Pr = 5.85 \times 10^{-10} \cdot 6.01 = 3.50 \times 10^{-9}\ mg/kg$$

Time Period	Effect	Plant Concentration due to Root Uptake (Pr) (mg/kg)
Adult	Carcinogenic	3.50 x 10^{-9}
Adult	Noncarcinogenic	2.10 x 10^{-8}
Child	Carcinogenic	2.10 x 10^{-8}
Child	Noncarcinogenic	2.10 x 10^{-8}
Infant	Carcinogenic	2.10 x 10^{-8}
Infant	Noncarcinogenic	2.10 x 10^{-8}

The concentration of vinyl chloride in below ground vegetables due to root uptake was calculated using Equation D-30.

$$Pr_{bg} = \frac{Cs \cdot RCF \cdot VG_{rootveg}}{Kd_s} \qquad \text{Eq. D-30}$$

where

Pr_{bg}	=	vinyl chloride concentration in plant due to root uptake from soil (mg/kg)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
$VG_{rootveg}$	=	correction factor for below-ground produce (1 dimensionless)
RCF	=	root concentration factor (9.09 µg vinyl chloride/g plant)/(µg vinyl chloride/ mℓ soil water)
Kd_s	=	soil-water partition coefficient (0.037 mℓ water/g soil)

$$Pr_{bg} = \frac{5.82 \cdot 10^{-10} \cdot 9.09 \cdot 1}{0.037} = 1.43 \cdot 10^{-7} \frac{mg}{kg}$$

Time Period	Effect	Below Ground Plant Concentration due to Root Uptake (Pr_{bg}) (mg/kg)
Adult	Carcinogenic	1.43 x 10^{-7}
Adult	Noncarcinogenic	8.57 x 10^{-7}
Child	Carcinogenic	8.57 x 10^{-7}
Child	Noncarcinogenic	8.57 x 10^{-7}
Infant	Carcinogenic	8.57 x 10^{-7}
Infant	Noncarcinogenic	8.57 x 10^{-7}

E.6 ANIMAL FEED CONCENTRATION

The concentration of vinyl chloride in animal feed was calculated using the same equations that were used to calculate the vinyl chloride concentrations in produce for human consumption. Forage and silage were treated as exposed produce while grain was treated as protected produce. The concentration of vinyl chloride in forage due to air to direct deposition was calculated using Equation D-27.

$$Pd = \frac{1000 \cdot Q \cdot (1.0 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - exp(-kp \cdot Tp)]}{Yp \cdot kp} \qquad \text{Eq. D-27}$$

where

Pd	=	vinyl chloride concentration in plant due to direct deposition (mg/kg)
1000	=	unit conversion factor (mg/g)
Q	=	vinyl chloride stack emission rate (1 g/s)
$Dydp$	=	adjusted dry deposition from particle phase (2.12 x 10^{-4} s/m^2-yr)
Fw	=	fraction of wet deposition that adheres to plant (0.6 dimensionless)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
$Dywp$	=	adjusted wet deposition from particle phase (0 s/m^2-yr)
Rp_{forage}	=	interception fraction of edible portion of plant (0.5 dimensionless)
kp	=	plant surface loss coefficient (18 yr^{-1})

Tp_{forage}	=	length of plant exposure to deposition of edible portion of plant, per harvest (0.12 yr)
Yp_{forage}	=	yield or standing crop biomass of the edible portion of the plant (0.24 kg/m^2)

$$Pd = \frac{1000 \cdot 1 \cdot (1.0 - 1) \cdot \left[2.12 \cdot 10^{-4} + (0.6 \cdot 0)\right] \cdot 0.5 \cdot [1.0 - exp(-18 \cdot 0.12)]}{0.24 \cdot 18} = 0 \frac{mg}{kg}$$

The concentration of vinyl chloride in forage due to air to plant transfer was calculated using Equation D-28.

$$Pv = Q \cdot F_V \cdot \frac{Cyv \cdot Bv_{ag} \cdot VG_{forage}}{\rho_a} \qquad \text{Eq. D-28}$$

where

Pv	=	vinyl chloride concentration in the plant due to air-to-plant transfer (mg/kg)
Q	=	vinyl chloride stack emission rate (1 g/s)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
Cyv	=	adjusted vapor phase air concentration (1.52 x 10^{-3} µg/m^3 per g/s)
VG_{forage}	=	forage correction factor (1 dimensionless)
Bv_{ag}	=	air-to-plant biotransfer factor (6.41 x 10^{-5} [mg pollutant/g plant tissue]/[mg vinyl chloride/g air])
ρ_a	=	density of air (1,200 g/m^3)

$$Pv = 1 \cdot 1 \cdot \frac{1.52 \cdot 10^{-3} \cdot 6.41 \cdot 10^{-5} \cdot 1}{1{,}200} = 8.12 \cdot 10^{-11} \frac{mg}{kg}$$

The concentration of vinyl chloride in animal feed due to root uptake was calculated using Equation D-29.

$$Pr = Cs \cdot Br_{ag} \qquad \text{Eq. D-29}$$

where

Pr	=	vinyl chloride concentration in plant due to root uptake from soil (mg/kg)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Br_{ag}	=	plant-to-soil bioconcentration factor for forage (6.01 dimensionless)

$$Pr = 5.82 \times 10^{-10} \cdot 6.01 = 3.50 \times 10^{-9} \; mg/kg$$

Time Period	Effect	Animal Feed Concentration due to Root Uptake (Pr) (mg/kg)
Adult	Carcinogenic	3.50×10^{-9}
Adult	Noncarcinogenic	2.10×10^{-8}
Child	Carcinogenic	2.10×10^{-8}
Child	Noncarcinogenic	2.10×10^{-8}
Infant	Carcinogenic	2.10×10^{-8}
Infant	Noncarcinogenic	2.10×10^{-8}

The concentration of vinyl chloride in silage due to air to direct deposition was calculated using Equation D-27.

$$Pd = \frac{1000 \cdot Q \cdot (1.0 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - exp(-kp \cdot Tp)]}{Yp \cdot kp} \qquad \text{Eq. D-27}$$

where

Pd	=	vinyl chloride concentration in plant due to direct deposition (mg/kg)
1000	=	unit conversion factor (mg/g)
Q	=	vinyl chloride stack emission rate (1 g/s)
$Dydp$	=	adjusted dry deposition from particle phase (2.12×10^{-4} s/m^2-yr)
Fw	=	fraction of wet deposition that adheres to plant (0.6 dimensionless)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
$Dywp$	=	adjusted wet deposition from particle phase (0 s/m^2-yr)
Rp_{silage}	=	interception fraction of edible portion of plant (0.46 dimensionless)
kp	=	plant surface loss coefficient (18 yr^{-1})
Tp_{silage}	=	length of plant exposure to deposition of edible portion of plant, per harvest (0.16 yr)
Yp_{silage}	=	yield or standing crop biomass of the edible portion of the plant (0.8 kg/m^2)

$$Pd = \frac{1000 \cdot 1 \cdot (1.0 - 1) \cdot [2.12 \cdot 10^{-4} + (0.6 \cdot 0)] \cdot 0.46 \cdot [1.0 - exp(-18 \cdot 0.16)]}{0.8 \cdot 18} = 0 \frac{mg}{kg}$$

The concentration of vinyl chloride in silage due to air to plant transfer was calculated using Equation D-28.

$$Pv = Q \cdot F_V \cdot \frac{Cyv \cdot Bv_{ag} \cdot VG_{silage}}{\rho_a} \qquad \text{Eq. D-28}$$

where

Pv	=	vinyl chloride concentration in the plant due to air-to-plant transfer (mg/kg)
Q	=	vinyl chloride stack emission rate (1 g/s)
F_v	=	fraction of air concentration in vapor phase (1 dimensionless)
Cyv	=	adjusted vapor phase air concentration (1.52×10^{-3} µg/m^3 per g/s)

VG_{silage}	=	silage correction factor (0.5 dimensionless)
Bv_{ag}	=	air-to-plant biotransfer factor (6.41 x 10^{-5} [mg pollutant/g plant tissue]/[mg vinyl chloride/g air])
ρ_a	=	density of air (1,200 g/m^3)

$$Pv = 1 \cdot 1 \cdot \frac{1.52 \cdot 10^{-3} \cdot 6.41 \cdot 10^{-5} \cdot 0.5}{1200} = 4.06 \cdot 10^{-11}\,\frac{mg}{kg}$$

The total concentration of vinyl chloride in each of the animal feeds was calculated as the sum of the vinyl chloride concentrations from the applicable mechanisms. The total vinyl chloride concentrations in each animal feed are summarized below:

$$Grain \quad P_{total} = Pr = 3.50 \cdot 10^{-9}\,\frac{mg}{kg}$$

$$Forage \quad P_{total} = Pr + Pd + Pv = 3.50 \cdot 10^{-9} + 0 + 8.12 \cdot 10^{-11} = 3.58 \cdot 10^{-9}\,\frac{mg}{kg}$$

$$Silage \quad P_{total} = Pr + Pd + Pv = 3.50 \cdot 10^{-9} + 0 + 4.06 \cdot 10^{-11} = 3.59 \cdot 10^{-9}\,\frac{mg}{kg}$$

Time Period	Effect	Grain Concentration (mg/kg)	Forage Concentration (mg/kg)	Silage Concentration (mg/kg)
Adult	Carcinogenic	3.50 x 10^{-9}	3.58 x 10^{-9}	3.54 x 10^{-9}
Adult	Noncarcinogenic	2.10 x 10^{-8}	2.11 x 10^{-8}	2.10 x 10^{-8}
Child	Carcinogenic	2.10 x 10^{-8}	2.11 x 10^{-8}	2.10 x 10^{-8}
Child	Noncarcinogenic	2.10 x 10^{-8}	2.11 x 10^{-8}	2.10 x 10^{-8}
Infant	Carcinogenic	2.10 x 10^{-8}	2.11 x 10^{-8}	2.10 x 10^{-8}
Infant	Noncarcinogenic	2.10 x 10^{-8}	2.11 x 10^{-8}	2.10 x 10^{-8}

E.7 ANIMAL PRODUCT CONCENTRATIONS

The concentration of vinyl chloride in animal products (meat, milk, and eggs) was calculated from the uptake of contaminated feed and soil. Vinyl chloride concentrations were calculated for beef, pork, poultry, eggs, and cow's milk. The concentration of vinyl chloride in beef was calculated using Equation D-31.

$$A_{beef} = \left(\sum_i \left(F_i \cdot Qp_i \cdot P_{total,i} \right) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{beef} \cdot MF \qquad \text{Eq. D-31}$$

where

A_{beef}	=	concentration of vinyl chloride in beef tissue (mg/kg)
F_i	=	fraction of plant type i grown on contaminated soil (1 dimensionless)
Qp_i	=	animal consumption rate of plant type i (8.8 (forage), 2.5 (silage), and 0.47 (grain) kg/day)
$P_{total,i}$	=	total concentration of vinyl chloride in plant type i (3.58 x 10^{-9} (forage), 3.54 x 10^{-9} (silage), and 3.50 x 10^{-9} (grain) mg/kg [carcinogenic effects, adult portion]; 2.11 x 10^{-8} (forage), 2.10 x 10^{-8}

		(silage), and 2.10 x 10^{-8} (grain) mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Qs	=	animal consumption rate of soil (0.5 kg soil/day)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Ba_{beef}	=	biotransfer factor for beef (1.05 x 10^{-3} day/kg)
Bs	=	soil bioavailability factor (1 dimensionless)
MF	=	metabolism factor (1 dimensionless)

$$A_{beef} = \left(\left(1 \cdot 8.8 \cdot 3.58 \cdot 10^{-9}\right) + \left(1 \cdot 2.5 \cdot 3.54 \cdot 10^{-9}\right) + \left(1 \cdot 0.47 \cdot 3.50 \cdot 10^{-9}\right) + 0.5 \cdot 5.82 \cdot 10^{-10} \cdot 1\right) \cdot 1.05 \cdot 10^{-3} \cdot 1$$

$$= 4.44 \cdot 10^{-11} \frac{mg}{kg}$$

Time Period	Effect	Beef Concentration (A_{beef}) (mg/kg)
Adult	Carcinogenic	4.44 x 10^{-11}
Adult	Noncarcinogenic	2.62 x 10^{-10}
Child	Carcinogenic	2.62 x 10^{-10}
Child	Noncarcinogenic	2.62 x 10^{-10}
Infant	Carcinogenic	2.62 x 10^{-10}
Infant	Noncarcinogenic	2.62 x 10^{-10}

The concentration of vinyl chloride in pork was calculated using Equation D-32.

$$A_{pork} = \left(\sum_i \left(F_i \cdot Qp_i \cdot P_{total,i}\right) + Qs \cdot Cs \cdot Bs\right) \cdot Ba_{pork} \cdot MF \qquad \text{Eq. D-32}$$

where

A_{pork}	=	concentration of vinyl chloride in pork tissue (mg/kg)
F_i	=	fraction of plant type i grown on contaminated soil (1 dimensionless)
Qp_i	=	animal consumption rate of plant type i (1.4 (silage) and 3.3 (grain) kg/day)
$P_{total,i}$	=	total concentration of vinyl chloride in plant type i (3.54 x 10^{-9} (silage) and 3.50 x 10^{-9} (grain) mg/kg [carcinogenic effects, adult portion]; 2.10 x 10^{-8} (silage) and 2.10 x 10^{-8} (grain) mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Qs	=	animal consumption rate of soil (0.37 kg soil/day)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Ba_{pork}	=	biotransfer factor for pork (1.28 x 10^{-3} day/kg)
Bs	=	soil bioavailability factor (1 dimensionless)
MF	=	metabolism factor (1 dimensionless)

$$A_{pork} = ((1 \cdot 1.4 \cdot 3.54 \cdot 10^{-9}) + (1 \cdot 3.3 \cdot 3.50 \cdot 10^{-9}) + 0.37 \cdot 5.82 \cdot 10^{-10} \cdot 1) \cdot 1.28 \cdot 10^{-3} \cdot 1$$
$$= 2.14 \cdot 10^{-11} \frac{mg}{kg}$$

Time Period	Effect	Pork Concentration (A_{pork}) (mg/kg)
Adult	Carcinogenic	2.14 x 10^{-11}
Adult	Noncarcinogenic	1.28 x 10^{-10}
Child	Carcinogenic	1.28 x 10^{-10}
Child	Noncarcinogenic	1.28 x 10^{-10}
Infant	Carcinogenic	1.28 x 10^{-10}
Infant	Noncarcinogenic	1.28 x 10^{-10}

The concentration of vinyl chloride in cow's milk was calculated using Equation D-33.

$$A_{milk} = \left(\sum_i (F_i \cdot Qp_i \cdot P_{total,i}) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{milk} \cdot MF \qquad \text{Eq. D-33}$$

where

A_{milk}	=	concentration of vinyl chloride in dairy milk (mg/kg)
F_i	=	fraction of plant type i grown on contaminated soil and eaten by the animal (1 dimensionless)
Qp_i	=	animal consumption rate of plant type i (13.2 (forage), 4.1 (silage), and 3 (grain) kg plant tissue/day)
$P_{total,i}$	=	total concentration of vinyl chloride in plant type i (3.58 x 10^{-9} (forage), 3.54 x 10^{-9} (silage), and 3.50 x 10^{-9} (grain) mg/kg [carcinogenic effects, adult portion]; 2.11 x 10^{-8} (forage), 2.10 x 10^{-8} (silage), and 2.10 x 10^{-8} (grain) mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Qs	=	animal consumption rate of soil (0.4 kg soil/day)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Ba_{milk}	=	biotransfer factor for milk (2.22 x 10^{-4} day/kg)
Bs	=	soil bioavailability factor (1 dimensionless)
MF	=	metabolism factor (1 dimensionless)

$$A_{milk} = ((1 \cdot 13.2 \cdot 3.58 \cdot 10^{-9}) + (1 \cdot 4.1 \cdot 3.54 \cdot 10^{-9}) + (1 \cdot 3 \cdot 3.50 \cdot 10^{-9}) + 0.4 \cdot 5.82 \cdot 10^{-10} \cdot 1)$$
$$\cdot 2.22 \cdot 10^{-4} \cdot 1 = 1.61 \cdot 10^{-11} \frac{mg}{kg}$$

Time Period	Effect	Dairy Milk Concentration (A_{milk}) (mg/kg)
Adult	Carcinogenic	1.61×10^{-11}
Adult	Noncarcinogenic	9.52×10^{-11}
Child	Carcinogenic	9.52×10^{-11}
Child	Noncarcinogenic	9.52×10^{-11}
Infant	Carcinogenic	9.52×10^{-11}
Infant	Noncarcinogenic	9.52×10^{-11}

The vinyl chloride concentration in poultry meat was calculated using Equation D-36.

$$A_{chick} = ((F \cdot Qp \cdot P_{total}) + Qs \cdot Cs \cdot Bs) \cdot Ba_{chick} \qquad \text{Eq. D-36}$$

where

A_{chick}	=	concentration of vinyl chloride in poultry meat (mg/kg)
F	=	fraction of grain grown on contaminated soil (1 dimensionless)
Qp	=	animal consumption rate of grain (0.2 kg/day)
P_{total}	=	total concentration of vinyl chloride in grain (3.50×10^{-9} mg/kg [carcinogenic effects, adult portion], 2.10×10^{-8} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Qs	=	animal consumption rate of soil (0.022 kg soil/day)
Cs	=	vinyl chloride concentration in soil (5.82×10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49×10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Ba_{chick}	=	biotransfer factor for poultry (7.76×10^{-4} day/kg)
Bs	=	soil bioavailability factor (1 dimensionless)

$$A_{chick} = ((1 \cdot 0.2 \cdot 3.50 \cdot 10^{-9}) + 0.022 \cdot 5.82 \cdot 10^{-10} \cdot 1) \cdot 7.76 \cdot 10^{-4} = 5.53 \cdot 10^{-13} \frac{mg}{kg}$$

Time Period	Effect	Poultry Concentration (A_{chick}) (mg/kg)
Adult	Carcinogenic	5.53×10^{-13}
Adult	Noncarcinogenic	3.32×10^{-12}
Child	Carcinogenic	3.32×10^{-12}
Child	Noncarcinogenic	3.32×10^{-12}
Infant	Carcinogenic	3.32×10^{-12}
Infant	Noncarcinogenic	3.32×10^{-12}

The vinyl chloride concentration in poultry eggs was calculated using Equation D-37.

$$A_{egg} = ((F \cdot Qp \cdot P_{total}) + Qs \cdot Cs \cdot Bs) \cdot Ba_{egg} \qquad \text{Eq. D-37}$$

where

A_{egg}	=	concentration of vinyl chloride in poultry eggs (mg/kg)
F	=	fraction of grain grown on contaminated soil (1 dimensionless)
Qp	=	animal consumption rate of grain (0.2 kg/day)
P_{total}	=	total concentration of vinyl chloride in grain (3.50 x 10^{-9} mg/kg [carcinogenic effects, adult portion], 2.10 x 10^{-8} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Qs	=	animal consumption rate of soil (0.022 kg soil/day)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Ba_{egg}	=	biotransfer factor for eggs (4.44 x 10^{-4} day/kg)
Bs	=	soil bioavailability factor (1 dimensionless)

$$A_{egg} = \left(\left(1 \cdot 0.2 \cdot 3.50 \cdot 10^{-9}\right) + 0.022 \cdot 5.82 \cdot 10^{-10} \cdot 1\right) \cdot 4.44 \cdot 10^{-4} = 3.16 \cdot 10^{-13} \frac{mg}{kg}$$

Time Period	Effect	Egg Concentration (A_{egg}) (mg/kg)
Adult	Carcinogenic	3.16 x 10^{-13}
Adult	Noncarcinogenic	1.90 x 10^{-12}
Child	Carcinogenic	1.90 x 10^{-12}
Child	Noncarcinogenic	1.90 x 10^{-12}
Infant	Carcinogenic	1.90 x 10^{-12}
Infant	Noncarcinogenic	1.90 x 10^{-12}

The vinyl chloride concentration in fish was calculated using Equation D-34.

$$C_{fish} = C_{dw} \cdot BCF_{fish} \qquad \text{Eq. D-34}$$

where

C_{fish}	=	vinyl chloride concentration in fish (mg/kg)
C_{dw}	=	vinyl chloride concentration in the dissolved water phase (1.76 x 10 ^{5} mg/ℓ)
BCF_{fish}	=	bioconcentration factor (2.39 ℓ/kg)

$$C_{fish} = 1.76 \cdot 10^{-5} \cdot 2.39 = 4.21 \cdot 10^{-5} \frac{mg}{kg}$$

E.8 QUANTIFICATION OF DIRECT EXPOSURE

Direct exposures to vinyl chloride were calculated as inhalation exposure concentrations for the infant, child, and adult portions of the subsistence fisher lifetime (I) exposure scenario. The inhalation exposure concentrations are time-weighted average concentrations derived from the modeled contaminant concentrations in air and adjusted based on the characteristics of the exposure scenario being evaluated. For the exposure scenario presented in these example calculations, the 5 years of direct inhalation exposure occur for the adult and during childhood. For the infant, direct inhalation exposure occurs for 1 year.

The vinyl chloride inhalation exposure concentration (direct exposure pathway) was calculated using Equation D-39. The calculation for the child carcinogenic effects are shown below followed by a summary table of the results for adult and infant carcinogenic effects as well as both infant, child, and adult noncarcinogenic effects.

$$EC = \frac{C_{(air)} \cdot ET \cdot EF \cdot ED}{AT \cdot 8760} \qquad \text{Eq. D-39}$$

where

EC	= inhalation exposure concentration to vinyl chloride (µg/m^3)
$C_{(air)}$	= AERMOD-calculated vinyl chloride air concentration (1.52 x 10^{-3} µg/m^3)
ET	= exposure time (24 hours/day)
EF	= exposure frequency (350 days/yr)
ED	= exposure duration (5 yr [adult and child], 1 yr [infant])
AT	= averaging time (78 yr [carcinogenic effects], 5 yr [noncarcinogenic effects adult and child portion], 1 yr [noncarcinogenic effects infant portion])
8,760	= unit conversion factor (hours/yr)

$$EC = \frac{1.52 \cdot 10^{-3} \cdot 24 \cdot 350 \cdot 5}{78 \cdot 8{,}760} = 9.34 \cdot 10^{-5}\ \frac{\mu g}{m3}$$

Time Period	Effect	Inhalation Exposure Concentration (*EC*) (µg/m^3)
Adult	Carcinogenic	9.34 x 10^{-5}
Adult	Noncarcinogenic	1.46 x 10^{-3}
Child	Carcinogenic	9.34 x 10^{-5}
Child	Noncarcinogenic	1.46 x 10^{-3}
Infant	Carcinogenic	1.87 x 10^{-5}
Infant	Noncarcinogenic	1.46 x 10^{-3}

NA - not applicable to this example exposure scenario

E.9 QUANTIFICATION OF INDIRECT DAILY INTAKE

The indirect intake via ingestion and dermal contact occur for each portion of the exposure scenario based on the receptor-specific exposure parameters. Although exclusive use of receptor-specific and site-specific exposure parameters for intake equations would yield a more realistic assessment of potential exposures, default exposure parameters were utilized to a great extent in this assessment to produce a reasonable maximum exposure (RME) result. The following paragraphs show the calculations performed to determine daily intake of vinyl chloride from each indirect exposure pathway.

Intake of vinyl chloride via incidental ingestion of contaminated soil was calculated using Equation D-40.

$$I_{soil} = Cs \cdot CR_{soil} \cdot F_{soil} \qquad \text{Eq. D-40}$$

where

I_{soil}	=	daily intake of vinyl chloride from soil (mg/day)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{soil}	=	consumption rate of soil (0.0001 kg/day [adult], 0.0002 kg/day [infant and child])
F_{soil}	=	fraction of consumed soil that is contaminated (1 dimensionless)

$$I_{soil} = 5.82 \cdot 10^{-10} \cdot 0.0001 \cdot 1 = 5.82 \cdot 10^{-14} \frac{mg}{day}$$

Time Period	Effect	Soil Ingestion Intake (I_{soil}) (mg/day)
Adult	Carcinogenic	5.82 x 10^{-14}
Adult	Noncarcinogenic	3.49 x 10^{-13}
Child	Carcinogenic	6.98 x 10^{-13}
Child	Noncarcinogenic	6.98 x 10^{-13}
Infant	Carcinogenic	6.98 x 10^{-13}
Infant	Noncarcinogenic	6.98 x 10^{-13}

Intake of vinyl chloride via ingestion of fruits and vegetables was calculated using Equation D-41.

$$I_{ag} = [((Pd + Pv + Pr) \cdot CR_{ag} + (Pr \cdot CR_{pp})) \cdot F_{ag} + (Pr_{bg} \cdot CR_{bg}) \cdot F_{bg}] \qquad \text{Eq. D-41}$$

where

I_{ag}	=	daily intake of vinyl chloride from fruits and vegetables (mg/day)
Pd	=	vinyl chloride concentration in above-ground fruits and vegetables due to direct deposition (0 mg/kg)
Pv	=	vinyl chloride concentration in above-ground fruits and vegetables due to air-to-plant transfer (8.12 x 10^{-11} mg/kg)
Pr	=	vinyl chloride concentration in above-ground fruits and vegetables due to root uptake (3.50 x 10^{-9} mg/kg [carcinogenic effects, adult portion], 2.10 x 10^{-8} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
Pr_{bg}	=	vinyl chloride concentration in below-ground vegetables due to root uptake (1.43 x 10^{-7} mg/kg [carcinogenic effects, adult portion], 8.57 x 10^{-7} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{ag}	=	consumption rate of above-ground exposed fruits and vegetables (0.560 (fruits) + 0.352 (vegetables) = 0.912 kg/day [adult], 0.469

		(fruits) + 0.118 (vegetables) = 0.587 kg/day [child], 0.303 (fruits +0.058 (vegetables) = 0.361 kg/day [infant])
CR_{pp}	=	consumption rate of above-ground protected fruits and vegetables (0.648 (fruits) + 0.248 (vegetables) = 0.896 kg/day [adult], 0.324 (fruits) + 0.098 (vegetables) = 0.422 kg/day [child], 0.065 (fruits) + 0.061 (vegetables) = 0.126 kg/day [infant])
F_{ag}	=	fraction of above-ground fruits and vegetables that are contaminated (0.4 dimensionless)
CR_{bg}	=	consumption rate of below-ground vegetables (0.328 kg/day [adult], 0.123 kg/day [child], 0.075 kg/day [infant])
F_{bg}	=	fraction of below-ground vegetables that is contaminated (0.4 dimensionless)

$$I_{ag} = \left[\left(\left(0 + 8.12 \cdot 10^{-11} + 3.50 \cdot 10^{-9}\right) \cdot 0.912 + \left(3.50 \cdot 10^{-9} \cdot 0.896\right)\right) \cdot 0.4 + \left(1.43 \cdot 10^{-7} \cdot 0.328\right) \cdot 0.4\right] = 2.13 \cdot 10^{-8} \frac{mg}{day}$$

Time Period	Effect	Produce Ingestion Intake (I_{ag}) (mg/day)
Adult	Carcinogenic	2.13×10^{-8}
Adult	Noncarcinogenic	1.28×10^{-7}
Child	Carcinogenic	5.07×10^{-8}
Child	Noncarcinogenic	5.07×10^{-8}
Infant	Carcinogenic	2.98×10^{-8}
Infant	Noncarcinogenic	2.98×10^{-8}

Intake of vinyl chloride via ingestion of contaminated beef was calculated using Equation D-42.

$$I_{beef} = A_{beef} \cdot CR_{beef} \cdot F_{beef} \qquad \text{Eq. D-42}$$

where

I_{beef}	=	daily intake of vinyl chloride from beef (mg/day)
A_{beef}	=	vinyl chloride concentration in beef tissue (4.44×10^{-11} mg/kg [carcinogenic effects, adult portion], 2.62×10^{-10} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{beef}	=	consumption rate of beef (0.157 kg/day [adult], 0.052 kg/day [child], 0.014 kg/day [infant])
F_{beef}	=	fraction of consumed beef that is contaminated (0.4 dimensionless)

$$I_{beef} = 4.44 \cdot 10^{-11} \cdot 0.157 \cdot 0.4 = 2.79 \cdot 10^{-12} \frac{mg}{day}$$

Time Period	Effect	Beef Ingestion Intake (I_{beef}) (mg/day)
Adult	Carcinogenic	2.79×10^{-12}
Adult	Noncarcinogenic	1.65×10^{-11}
Child	Carcinogenic	5.45×10^{-12}
Child	Noncarcinogenic	5.45×10^{-12}
Infant	Carcinogenic	1.47×10^{-12}
Infant	Noncarcinogenic	1.47×10^{-12}

Intake of vinyl chloride via ingestion of contaminated pork was calculated using Equation D-43.

$$I_{pork} = A_{pork} \cdot CR_{pork} \cdot F_{pork} \qquad \text{Eq. D-43}$$

where

I_{pork} = daily intake of vinyl chloride from pork (mg/day)
A_{pork} = vinyl chloride concentration in pork tissue (2.14×10^{-11} mg/kg [carcinogenic effects, adult portion], 1.28×10^{-10} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{pork} = consumption rate of pork (0.073 kg/day [adult], 0.024 kg/day [child], 0.005 kg/day [infant])
F_{pork} = fraction of consumed pork that is contaminated (0.4 dimensionless)

$$I_{pork} = 2.14 \cdot 10^{-11} \cdot 0.073 \cdot 0.4 = 6.25 \cdot 10^{-13} \frac{mg}{day}$$

Time Period	Effect	Pork Ingestion Intake (I_{pork}) (mg/day)
Adult	Carcinogenic	6.25×10^{-13}
Adult	Noncarcinogenic	3.74×10^{-12}
Child	Carcinogenic	1.23×10^{-12}
Child	Noncarcinogenic	1.23×10^{-12}
Infant	Carcinogenic	2.56×10^{-13}
Infant	Noncarcinogenic	2.56×10^{-13}

Intake of vinyl chloride via ingestion of contaminated poultry was calculated using Equation D-47.

$$I_{chick} = A_{chick} \cdot CR_{chick} \cdot F_{chick} \qquad \text{Eq. D-47}$$

where

I_{chick} = daily intake of vinyl chloride from poultry meat (mg/day)
A_{chick} = vinyl chloride concentration in poultry meat (5.53×10^{-13} mg/kg [carcinogenic effects, adult portion], 3.32×10^{-12} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{chick} = consumption rate of poultry (0.124 kg/day [adult], 0.047 kg/day [child], 0.023 kg/day [infant])

F_{chick} = fraction of consumed poultry that is contaminated (0.4 dimensionless)

$$I_{chick} = 5.53 \cdot 10^{-13} \cdot 0.124 \cdot 0.4 = 2.74 \cdot 10^{-14} \frac{mg}{day}$$

Time Period	Effect	Poultry Ingestion Intake (I_{chick}) (mg/day)
Adult	Carcinogenic	2.74×10^{-14}
Adult	Noncarcinogenic	1.65×10^{-13}
Child	Carcinogenic	6.25×10^{-14}
Child	Noncarcinogenic	6.25×10^{-14}
Infant	Carcinogenic	3.05×10^{-14}
Infant	Noncarcinogenic	3.05×10^{-14}

Intake of vinyl chloride via ingestion of contaminated eggs was calculated using Equation D-46.

$$I_{egg} = A_{egg} \cdot CR_{egg} \cdot F_{egg} \qquad \text{Eq. D-46}$$

where

I_{egg} = daily intake of vinyl chloride from eggs (mg/day)
A_{egg} = vinyl chloride concentration in eggs (3.16×10^{-13} mg/kg [carcinogenic effects, adult portion], 1.90×10^{-12} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{egg} = consumption rate of eggs (0.070 kg/day [adult], 0.032 kg/day [child], 0.010 kg/day [infant])
F_{egg} = fraction of consumed eggs that are contaminated (0.4 dimensionless)

$$I_{egg} = 3.16 \cdot 10^{-13} \cdot 0.070 \cdot 0.4 = 8.85 \cdot 10^{-15} \frac{mg}{day}$$

Time Period	Effect	Egg Ingestion Intake (I_{egg}) (mg/day)
Adult	Carcinogenic	8.85×10^{-15}
Adult	Noncarcinogenic	5.32×10^{-14}
Child	Carcinogenic	2.43×10^{-14}
Child	Noncarcinogenic	2.43×10^{-14}
Infant	Carcinogenic	7.62×10^{-15}
Infant	Noncarcinogenic	7.62×10^{-15}

Intake of vinyl chloride via ingestion of contaminated dairy milk was calculated using Equation D-44.

$$I_{milk} = A_{milk} \cdot CR_{milk} \cdot F_{milk} \qquad \text{Eq. D-44}$$

where

I_{milk}	=	daily intake of vinyl chloride from dairy milk (mg/day)
A_{milk}	=	vinyl chloride concentration in dairy milk (1.61x 10^{-11} mg/kg [carcinogenic effects, adult portion], 9.52 x 10^{-11} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
CR_{milk}	=	consumption rate of dairy milk (0.993 kg/day [adult], 1.052 kg/day [child], 0.380 kg/day [infant])
F_{milk}	=	fraction of consumed dairy milk that is contaminated (0.4 dimensionless)

$$I_{milk} = 1.61 \cdot 10^{-11} \cdot 0.993 \cdot 0.4 = 6.39 \cdot 10^{-12} \frac{mg}{day}$$

Time Period	Effect	Dairy Milk Ingestion Intake (I_{milk}) (mg/day)
Adult	Carcinogenic	6.39 x 10^{-12}
Adult	Noncarcinogenic	3.78 x 10^{-11}
Child	Carcinogenic	4.01 x 10^{-11}
Child	Noncarcinogenic	4.01 x 10^{-11}
Infant	Carcinogenic	1.45 x 10^{-11}
Infant	Noncarcinogenic	1.45 x 10^{-11}

Intake of vinyl chloride via ingestion of contaminated fish was calculated using Equation D-45.

$$I_{fish} = C_{fish} \cdot CR_{fish} \cdot F_{fish} \qquad \text{Eq. D-45}$$

where

I_{fish}	=	daily intake of vinyl chloride from fish (mg/day)
C_{fish}	=	vinyl chloride concentration in fish (4.21 x 10^{-5} mg/kg)
CR_{fish}	=	consumption rate of fish (0.168 kg/day [adult], 0.067 kg/day [child], 0.023 kg/day [infant])
F_{fish}	=	fraction of consumed fish that is contaminated (1.0 dimensionless)

$$I_{fish} = 4.21 \cdot 10^{-5} \cdot 0.168 \cdot 1 = 7.07 \cdot 10^{-6} \frac{mg}{day}$$

Time Period	Effect	Fish Ingestion Intake (I_{fish}) (mg/day)
Adult	Carcinogenic	7.07 x 10^{-6}
Adult	Noncarcinogenic	7.07 x 10^{-6}
Child	Carcinogenic	2.82 x 10^{-6}
Child	Noncarcinogenic	2.82 x 10^{-6}
Infant	Carcinogenic	9.68 x 10^{-7}
Infant	Noncarcinogenic	9.68 x 10^{-7}

Intake of vinyl chloride via incidental ingestion of contaminated surface water due to swimming was calculated for the adult and child portions using Equation D-48.

$$I_{sw} = \frac{C_{wctot} \cdot CR_{sw} \cdot F_{sw} \cdot EF}{1000 \cdot 365} \quad \text{Eq. D-48}$$

where

I_{sw} = daily intake of vinyl chloride from incidental ingestion of surface water (mg/day)
C_{wctot} = total vinyl chloride concentration in water column (1.76 x 10^{-5} mg/ℓ)
CR_{sw} = rate of consumption of surface water (71 mℓ/hr [adult], 120 mℓ/hr [child])
F_{sw} = swimming frequency (3 hr/day)
EF = exposure frequency (12 days/yr)
365 = conversion factor (days/yr)
1000 = conversion factor (*mℓ/ℓ*)

$$I_{sw} = \frac{1.76 \cdot 10^{-5} \cdot 71 \cdot 3 \cdot 12}{1000 \cdot 365} = 1.23 \cdot 10^{-7} \frac{mg}{day}$$

Time Period	Effect	Incidental Ingestion of Surface Water (I_{SW}) (mg/day)
Adult	Carcinogenic	1.23 x 10^{-7}
Adult	Noncarcinogenic	1.23 x 10^{-7}
Child	Carcinogenic	2.08 x 10^{-7}
Child	Noncarcinogenic	2.08 x 10^{-7}
Infant	Carcinogenic	NA
Infant	Noncarcinogenic	NA

Vinyl chloride is not one of the COPCs that have been identified as a chemical possibly found in breast milk. Therefore, vinyl chloride was not included in the breast milk pathway of the MPHRA and not calculated as an intake pathway in this appendix.

Total daily vinyl chloride ingestion was calculated using Equation D-50.

$$I_{total} = I_{soil} + I_{ag} + I_{beef} + I_{pork} + I_{milk} + I_{fish} + I_{egg} + I_{chick} + I_{sw} + I_{bm} \quad \text{Eq. D-50}$$

where

I_{total} = total daily intake of vinyl chloride through ingestion (mg/day)
I_{soil} = daily intake of vinyl chloride from soil (result of Eq. D-40 for age group/effect combination)
I_{ag} = daily intake of vinyl chloride from fruits and vegetables (result of Eq. D-41 for age group/effect combination)
I_{beef} = daily intake of vinyl chloride from beef (result of Eq. D-42 for age group/effect combination)
I_{pork} = daily intake of vinyl chloride from pork (result of Eq. D-43 for age group/effect combination)

I_{milk}	=	daily intake of vinyl chloride from dairy milk (result of Eq. D-44 for age group/effect combination)
I_{fish}	=	daily intake of vinyl chloride from fish (result of Eq. D-45 for age group/effect combination)
I_{egg}	=	daily intake of vinyl chloride from eggs (result of Eq. D-46 for age group/effect combination)
I_{chick}	=	daily intake of vinyl chloride from poultry (result of Eq. D-47 for age group/effect combination)
I_{sw}	=	daily intake of vinyl chloride from incidental ingestion of surface water (result of Eq. D-48 for adult and child portions)
I_{bm}	=	daily intake of vinyl chloride from breast milk (0 mg/day for vinyl chloride)

$$I = 5.82 \cdot 10^{-14} + 2.13 \cdot 10^{-8} + 2.79 \cdot 10^{-12} + 6.25 \cdot 10^{-13} + 2.74 \cdot 10^{-14} + 8.85 \cdot 10^{-15} + 6.39 \cdot 10^{-12}$$
$$+ 7.07 \cdot 10^{-6} + 1.23 \cdot 10^{-7} + 0 = 7.21 \cdot 10^{-6} \frac{mg}{day}$$

Time Period	Effect	Total Daily Intake (I_{total}) (mg/day)
Adult	Carcinogenic	7.21×10^{-6}
Adult	Noncarcinogenic	7.32×10^{-6}
Child	Carcinogenic	3.08×10^{-6}
Child	Noncarcinogenic	3.08×10^{-6}
Infant	Carcinogenic	9.97×10^{-7}
Infant	Noncarcinogenic	9.97×10^{-7}

The average daily ingestion dose of vinyl chloride was calculated using Equation D-51.

$$I_{ingested} = \frac{I_{total} \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \qquad \text{Eq. D-51}$$

where

$I_{ingested}$	=	average daily ingestion dose (mg/kg of body weight-day)
I_{total}	=	total daily intake of chemical through ingestion, (result of Eq. D-50 for age group/effect combination)
EF	=	exposure frequency, (350 day/yr)
ED	=	exposure duration, (30 yr [adult], 5 yr [child], 1 yr [infant])
BW	=	body weight, (80 kg [adult], 16.2 kg [child], 7.8 kg [infant])
AT	=	averaging time, (78 yr [carcinogenic effects], 30 yr [noncarcinogenic effects adult portion], 5 yr [noncarcinogenic effects child portion], 1 yr [noncarcinogenic effects infant portion]))
365	=	conversion factor (day/yr)

$$I_{ingested} = \frac{7.21 \cdot 10^{-6} \cdot 350 \cdot 30}{80 \cdot 78 \cdot 365} = 3.32 \cdot 10^{-8} \frac{mg}{kg \cdot day}$$

Time Period	Effect	Daily Ingestion Dose ($I_{ingested}$) (mg/kg-day)
Adult	Carcinogenic	3.32×10^{-8}
Adult	Noncarcinogenic	8.77×10^{-8}
Child	Carcinogenic	1.17×10^{-8}
Child	Noncarcinogenic	1.82×10^{-7}
Infant	Carcinogenic	1.57×10^{-9}
Infant	Noncarcinogenic	1.23×10^{-7}

The dermal absorbed dose of vinyl chloride per swimming event was calculated using Equation D-52b.

$$DA_{event} = FA \cdot K_p \cdot C_{dw} \left[\frac{t_{event}}{1+B} + 2\tau_{event} \left(\frac{1+3B+3B^2}{(1+B)^2} \right) \right] \qquad \text{Eq. D-52b}$$

where

DA_{event} = dermally absorbed dose per event (mg/cm^2-event)
FA = fraction absorbed water (1 dimensionless)
K_p = dermal permeability coefficient of vinyl chloride in water (0.0056 cm/hr)
C_{dw} = vinyl chloride concentration in the dissolved water phase (1.76×10^{-8} mg/cm^3)
t_{event} = duration of the swimming event (3 hr/event)
τ_{event} = lag time per event (0.235 hr/event)
B = dimensionless ration of the permeability coefficient of vinyl chloride through the stratum corneum relative to its permeability across the viable epidermis (1.70×10^{-2} dimensionless)

$$DA_{event} = 1 \cdot 0.0056 \cdot 1.76 \cdot 10^{-8} \left[\frac{3}{1+1.70 \cdot 10^{-2}} + 2 \cdot 0.235 \left(\frac{1+3 \cdot 1.70 \cdot 10^{-2} + 3 \cdot (1.70 \cdot 10^{-2})^2}{(1+1.70 \cdot 10^{-2})^2} \right) \right]$$

$$= 3.38 \cdot 10^{-10} \frac{mg}{cm^2 \cdot event}$$

Dermal uptake of vinyl chloride from surface water was calculated for the adult and child portions using Equation D-53.

$$DAD_{water} = \frac{DA_{event} \cdot EV \cdot ED \cdot EF_{sw} \cdot SA}{BW \cdot AT \cdot 365} \qquad \text{Eq. D-53}$$

where

DAD_{water} = dermal absorbed dose (mg/kg of body weight-day)
DA_{event} = dermally absorbed dose per event (3.38×10^{-10} mg/cm^2-event)
SA = skin surface area available for contact (18,000 cm^2 [adult], 6,600 cm^2 [child])
EV = event frequency (1 events/day)

EF_{sw}	=	exposure frequency (12 days/yr)
ED	=	exposure duration (30 yr [adult], 5 yr [child])
BW	=	body weight (80 kg [adult], 16.2 kg [child])
AT	=	averaging time (78 yr [carcinogenic effects], 30 yr [noncarcinogenic effects adult portion], 5 yr [noncarcinogenic effects child portion])
365	=	conversion factor (day/yr)

$$DAD_{water} = \frac{3.38 \cdot 10^{-10} \cdot 1 \cdot 30 \cdot 12 \cdot 18{,}000}{80 \cdot 78 \cdot 365} = 9.61 \cdot 10^{-10} \frac{mg}{kg \cdot day}$$

Time Period	Effect	Dermal Absorbed Dose - Water (DAD_{water}) (mg/kg-day)
Adult	Carcinogenic	9.61×10^{-10}
Adult	Noncarcinogenic	2.50×10^{-9}
Child	Carcinogenic	2.90×10^{-10}
Child	Noncarcinogenic	4.53×10^{-9}
Infant	Carcinogenic	NA
Infant	Noncarcinogenic	NA

NA - not applicable to this example exposure scenario

The dermal absorbed dose of vinyl chloride per soil contact event was calculated using Equation D-54.

$$DA_{event} = Cs \cdot 10^{-6} \cdot AF \cdot ABS_d \qquad \text{Eq. D-54}$$

DA_{event}	=	dermally absorbed dose per event (mg/cm^2-event)
Cs	=	vinyl chloride concentration in soil (5.82 x 10^{-10} mg/kg [carcinogenic effects, adult portion], 3.49 x 10^{-9} mg/kg [carcinogenic effects, infant and child portions; noncarcinogenic effects])
10^{-6}	=	conversion factor (kg/mg)
AF	=	soil adherence factor (0.07 mg/cm^2-event [adult], 0.20 mg/cm^2-event [child and infant])
ABS_d	=	dermal absorption fraction (0.1 dimensionless)

$$DA_{event} = 5.82 \cdot 10^{-10} \cdot 10^{-6} \cdot 0.07 \cdot 0.1 = 4.09 \cdot 10^{-18} \frac{mg}{cm^2 \cdot event}$$

Time Period	Effect	Dermal Absorbed Dose Per Event- Soil (DA_{event}) (mg/cm^2-event)
Adult	Carcinogenic	4.09×10^{-18}
Adult	Noncarcinogenic	2.45×10^{-17}
Child	Carcinogenic	7.01×10^{-17}
Child	Noncarcinogenic	7.01×10^{-17}
Infant	Carcinogenic	7.01×10^{-17}
Infant	Noncarcinogenic	7.01×10^{-17}

Dermal uptake of vinyl chloride from soil contact was calculated using Equation D-55.

$$DAD_{soil} = \frac{DA_{event} \cdot EV \cdot ED \cdot EF \cdot SA}{BW \cdot AT \cdot 365} \qquad \text{Eq. D-55}$$

where

DAD_{soil}	=	dermal absorbed dose from soil (mg/kg of body weight-day)
DA_{event}	=	dermally absorbed dose per event (result of Eq. D-54 for age group/effect combination)
SA	=	skin surface area available for contact (5,700 cm^2 [adult], 2,800 cm^2 [child], 2,625 cm^2 [infant])
EV	=	event frequency (1 events/day)
EF	=	exposure frequency (350 days/yr)
ED	=	exposure duration (30 yr [adult], 5 yr [child], 1 yr [infant])
BW	=	body weight (80 kg [adult], 16.2 kg [child], 7.8 kg [infant])
AT	=	averaging time (78 yr [carcinogenic effects], 30 yr [noncarcinogenic effects adult portion], 5 yr [noncarcinogenic effects child portion], 1 yr [noncarcinogenic effects infant portion])
365	=	conversion factor (day/yr)

$$DAD_{soil} = \frac{4.07 \cdot 10^{-18} \cdot 1 \cdot 30 \cdot 350 \cdot 5700}{80 \cdot 78 \cdot 365} = 1.07 \cdot 10^{-16} \frac{mg}{kg \cdot day}$$

Time Period	Effect	Dermal Absorbed Dose - Soil (DAD_{soil}) (mg/kg-day)
Adult	Carcinogenic	1.07×10^{-16}
Adult	Noncarcinogenic	1.68×10^{-15}
Child	Carcinogenic	7.44×10^{-16}
Child	Noncarcinogenic	1.16×10^{-14}
Infant	Carcinogenic	2.90×10^{-16}
Infant	Noncarcinogenic	2.26×10^{-14}

The total indirect exposure of vinyl chloride was calculated using Eq D-56.

$$I_{indirect} = I_{ingested} + DAD_{soil} + DAD_{water} \qquad \text{Eq. D-56}$$

where

$I_{indirect}$	=	total indirect exposure (mg/kg of body weight-day)
$I_{ingested}$	=	average daily ingestion dose (result of Eq. D-51 for age group/effect combination)
DAD_{soil}	=	dermal absorbed dose from soil (result of Eq. D-55 for age group/effect combination)
DAD_{water}	=	dermal absorbed dose from water (result of Eq. D-53 for age group/effect combination)

$$I_{indirect} = 3.32 \cdot 10^{-8} + 9.62 \cdot 10^{-10} + 1.07 \cdot 10^{-16} = 3.42 \cdot 10^{-8} \frac{mg}{kg \cdot day}$$

Time Period	Effect	Total Indirect Exposure ($I_{indirect}$) (mg/kg-day)
Adult	Carcinogenic	3.42 x 10^{-8}
Adult	Noncarcinogenic	9.02 x 10^{-8}
Child	Carcinogenic	1.20 x 10^{-8}
Child	Noncarcinogenic	1.87 x 10^{-7}
Infant	Carcinogenic	1.57 x 10^{-9}
Infant	Noncarcinogenic	1.23 x 10^{-7}

E.10 QUANTIFICATION OF EARLY-LIFE EXPOSURE

Some chemicals present increased risk if exposure occurs early in life. For these mutagenic chemicals (vinyl chloride, methylene chloride, and trichloroethene are the only mutagenic COPCs included in this MPHRA), a modified calculation procedure must be used to account for additional risk due to early-life exposure. This procedure partitions risk into segments that are calculated separately and summed together to determine total risk. The early-life portion of the risk is not pro-rated over the exposure duration and is summed with the pro-rated portions to determine the total risk from exposure to chemicals with mutagenic modes of action. The additional early-life vinyl chloride exposure concentration for carcinogenic effects was calculated for inhalation using Equation D-57a.

$$EC_{VC,earlylife} = \frac{[F_v \cdot Cyv + (1 - F_v) \cdot Cyp] \cdot ET \cdot EF}{365 \cdot 24} \quad \text{Eq. D-57a}$$

where

$EC_{VC,earlylife}$	=	additional early-life inhalation exposure concentration (µg/m^3)
F_v	=	fraction of air concentration in vapor phase (dimensionless), (1)
Cyv	=	vapor phase air concentration (1.52 x 10^{-3} µg/m^3), (modeled value)
Cyp	=	particle phase air concentration (1.50 x 10^{-3} µg/m^3), (modeled value)
ET	=	exposure time (24 hr/day)
EF	=	exposure frequency (365 day/yr)
365	=	unit conversion factor (day/yr)
24	=	unit conversion factor (hours/day)

$$EC_{VC,earlylife} = \frac{1.52 \cdot 10^{-3} \cdot 24 \cdot 365}{24 \cdot 365} = 1.52 \cdot 10^{-3} \frac{\mu g}{m3}$$

Because the lifetime(I) receptor includes indirect exposure starting as an infant and continuing through childhood, the vinyl chloride early-life exposure of indirect pathways is calculated as the time-weighted average of infant and child exposures over the total early-life exposure period.

EPA guidance[1] does not specify the duration during which increased risk due to early-life exposure may occur, other than stating "*Because the exact age window of susceptibility in humans is not known, but is likely to be much shorter in duration than 10 years…*" To provide a conservative estimate of the increased risk to vinyl chloride for the lifetime (I) exposure scenario, the early-life exposure period was assumed to occur over the first 6 years of life to correspond to the infant and child exposure periods. As such, the early-life exposure for carcinogenic effects of vinyl chloride was calculated for indirect pathways for the infant and child, using Equation D-57b, which were then averaged over the total early-life exposure period (6 years) as discussed below.

$$I_{indirect(earlylife,infant/child)} = \sum \frac{I_i \cdot EF}{BW \cdot 365} + \sum \frac{DA_{eventj} \cdot EV \cdot EF_j \cdot SA_j}{BW \cdot 365} \qquad \text{Eq. D-57b}$$

where

$I_{indirect(earlylife)}$	=	early-life indirect exposure to vinyl chloride for infant or child (mg/kg of body weight-day)
I_i	=	total daily intake of chemical through ingestion of media type i (mg/day), (calculated by Eq. D-40 through D-49)
EF	=	exposure frequency for ingestion (365 day/yr), (exposure scenario-specific value)
BW	=	body weight (7.8 kg for infant, 16.2 kg for child), (exposure scenario-specific value)
365	=	conversion factor (day/yr)
DA_{eventj}	=	dermally absorbed dose per dermal contact event of type j (mg/cm^2-event), (calculated by Eq. D-52a, D-52b, or D-54)
SA_j	=	skin surface area available for dermal contact of type j, (exposure scenario-specific value)
EV	=	event frequency (1 events/day), (site-specific value)
EF_j	=	exposure frequency for dermal contact of type j (365 days/yr for soil, 12 days/yr for water), (site-specific value)

Because the exposure frequency for ingestion and body weights do not change when calculationg the $I_{indirect(earlylife)}$ for either the infant or the child, Equation D-57b can be reduced to:

$$I_{indirect(earlylife,infant/child)} = \frac{\Sigma I_i \cdot EF}{BW \cdot 365} + \frac{\left[\left(DA_{soil} \cdot SA_{soil} \cdot EF_{soil}\right) + \left(DA_{water} \cdot SA_{water} \cdot EF_{water}\right)\right] \cdot EV}{BW \cdot 365}$$

where

ΣI_i	=	total daily intake of vinyl chloride through ingestion (mg/day) , (calculated by Eq. D-50), (9.97 x 10^{-7} for infant and 3.08 x 10^{-6} for child)
DA_{soil}	=	dermally absorbed dose per dermal contact event of soil (mg/cm^2-event), (7.01 x 10^{-17} for infant and child)

[1] Toxicological Review of Vinyl Chloride in Support of Summary Information on the Integrated Risk Information System (IRIS) (USEPA, 2000).

SA_{soil}	=	skin surface area available for dermal contact with soil (2,625 cm^2 for infant and 2,800 cm^2 for child)
EF_{soil}	=	exposure frequency for dermal contact with soil (365 days/yr for soil)
DA_{water}	=	dermally absorbed dose per dermal contact event of water for child only (3.38 x 10^{-10} mg/cm^2-event), (calculated by Eq. D-52b)
SA_{water}	=	skin surface area available for dermal contact with water (6,600 cm^2 for child)
EF_{water}	=	exposure frequency for dermal contact with water (12 days/yr)

Infant early-life indirect exposure to vinyl chloride is calculated as:

$$I_{indirect(earlylife,infant)} = \frac{9.98 \cdot 10^{-7} \cdot 365}{7.8 \cdot 365} + \frac{7.01 \cdot 10^{-17} \cdot 2{,}625 \cdot 365 \cdot 1}{7.8 \cdot 365} = 1.28 \cdot 10^{-7} \ \frac{mg}{kg \cdot day}$$

Child early-life indirect exposure to vinyl chloride is calculated as:

$$I_{indirect(earlylife,child)} = \frac{3.08 \cdot 10^{-6} \cdot 365}{16.2 \cdot 365} + \frac{\left[(7.01 \cdot 10^{-17} \cdot 2{,}800 \cdot 365) + (3.38 \cdot 10^{-10} \cdot 6{,}600 \cdot 12)\right] \cdot 1}{16.2 \cdot 365} = 1.95 \cdot 10^{-7} \ \frac{mg}{kg \cdot day}$$

The time-weighted average early-life exposure for the entire early-life exposure period (6 years) is calculated as:

$$I_{indirect(earlylife)} = \left(\frac{1}{6} \cdot I_{indrect(earlylife,infant)} + \frac{5}{6} \cdot I_{indrect(earlylife,child)}\right)$$

$$I_{indirect(earlylife)} = \left(\frac{1}{6} \cdot 1.28 \cdot 10^{-7} + \frac{5}{6} \cdot 1.95 \cdot 10^{-7}\right) = 1.84 \cdot 10^{-7} \ \frac{mg}{kg \cdot day}$$

E.11 QUANTIFICATION OF RISK AND HAZARD

Lifetime cancer risk and hazard were calculated by summing cancer risks and hazards during different stages of life (i.e., infant, child, adult). Exposure durations during each phase of life must add up to the total lifetime exposure duration. For this example (fisher lifetime (I) exposure scenario), the 30-year exposure duration for a fisher was apportioned for the following stages of life:

- additional early-life exposure
- exposure as an infant (1 year)
- exposure as a child (5 years)
- exposure as an adult (24 years)

E.11.1 CARCINOGENIC EFFECTS FROM DIRECT EXPOSURES

Cancer risk from direct exposure to (inhalation of) chemical emissions in air was calculated for COPCs with available inhalation unit risk factors. The cancer risk for vinyl chloride was calculated by multiplying the inhalation exposure concentration by the inhalation unit risk factor using Equation D-58:

$$Cancer\ Risk_D = \left(EC_{VC,earlylife} + EC_{infant} + \frac{4}{5} \cdot EC_{child} + EC_{adult} \right) \cdot IUR \qquad \text{Eq. D-58}$$

where

$Cancer\ Risk_D$	=	excess lifetime cancer risk via inhalation (dimensionless)
$EC_{VC,earlylife}$	=	additional early-life inhalation exposure concentration of vinyl chloride (μg/m^3), (calculated by Eq. D-57a) (1.52 x 10^{-3} μg/m^3)
EC_{infant}	=	inhalation exposure concentration of chemical as an infant (μg/m^3), (calculated by Eq. D-39) (1.87 x 10^{-5} μg/m^3)
EC_{child}	=	inhalation exposure concentration of chemical as a child (μg/m^3), (calculated by Eq. D-39) (9.34 x 10^{-5} μg/m^3)
EC_{adult}	=	inhalation exposure concentration of chemical as an adult (μg/m^3), (calculated by Eq. D-39) (0)
IUR	=	vinyl chloride inhalation unit risk (4.40 x 10^{-6} [μg/m^3]$^{-1}$)

$$Cancer\ Risk_D = \left(1.52 \cdot 10^{-3} + 1.87 \cdot 10^{-5} + \frac{4}{5} \cdot 9.34 \cdot 10^{-5} + 0 \right) \cdot 4.40 \cdot 10^{-6} = 7.09 \cdot 10^{-9}$$

E.11.2 CARCINOGENIC EFFECTS FROM INDIRECT EXPOSURES

Cancer risk from indirect exposure to vinyl chloride was calculated by multiplying the total indirect exposure from all life stages by the oral cancer slope factor using Equation D-59.

$$Cancer\ Risk_I = \left(I_{indirect(earlylife)} + I_{indirect(infant)} + I_{indirect(child)} + \frac{24}{30} \cdot I_{indirect(adult)} \right) \cdot CSF_O \qquad \text{Eq. D-59}$$

where

$Cancer\ Risk_I$	=	excess lifetime cancer risk from indirect exposures (dimensionless)
$I_{indirect(earlylife)}$	=	indirect exposure to mutagenic chemical during early life (not pro-rated over exposure duration) (1.84 x 10^{-7} mg/kg of body weight-day)
$I_{indirect(infant)}$	=	indirect exposure to chemical as an infant (1.57 x 10^{-9} mg/kg of body weight-day)
$I_{indirect(child)}$	=	indirect exposure to chemical as a child (1.20 x 10^{-8} mg/kg of body weight day)
$I_{indirect(adult)}$	=	indirect exposure to chemical as an adult (3.42 x 10^{-8} mg/kg of body weight-day)
CSF_O	=	oral cancer slope factor for chemical (7.20 x 10^{-1} [mg/kg of body weight-day]$^{-1}$)

$$Cancer\,Risk_i = \left(1.84 \cdot 10^{-7} + 1.57 \cdot 10^{-9} + 1.20 \cdot 10^{-8} + \frac{24}{30} \cdot 3.42 \cdot 10^{-8}\right) \cdot 7.20 \cdot 10^{-1} = 1.62 \cdot 10^{-7}$$

Overall cancer risk from exposure to vinyl chloride was calculated using Equation D-62.

$$Overall\,Cancer\,Risk = Total\,Cancer\,Risk_D + Total\,Cancer\,Risk_I \qquad \text{Eq. D-62}$$

where

Overall Cancer Risk	=	overall excess lifetime cancer risk via all routes of exposure (dimensionless)
Total Cancer Risk$_D$	=	total excess cancer risk via direct inhalation exposure (7.09×10^{-9})
Total Cancer Risk$_I$	=	total excess cancer risk via indirect exposures (1.62×10^{-7})

$$Overall\,Cancer\,Risk = 7.09 \cdot 10^{-9} + 1.62 \cdot 10^{-7} = 1.69 \cdot 10^{-7}$$

E.11.3 NONCARCINOGENIC EFFECTS FROM DIRECT AND INDIRECT EXPOSURES

For noncarcinogenic chemicals, a noncarcinogenic hazard quotient (HQ) is calculated by comparing the estimated exposure level over a specified time period (e.g., lifetime) with the appropriate non-cancer toxicity value (i.e., RfD). The noncarcinogenic HQ is the measure used to evaluate the potential for noncarcinogenic toxicity to occur in an individual. The noncarcinogenic HQ assumes that there is a level of exposure (e.g., RfD) below which it is unlikely for even sensitive subpopulations to experience adverse health effects.

Noncarcinogenic hazard from inhalation of vinyl chloride was calculated using Equation D-63.

$$HQ_D = \frac{\frac{1}{5} \cdot EC_{(infant)} + \frac{4}{5} \cdot EC_{(child)} + EC_{(adult)}}{(RfC \cdot 1{,}000)} \qquad \text{Eq. D-63}$$

where

HQ_D	=	HQ for direct inhalation exposure (dimensionless)
$EC_{(infant)}$	=	direct inhalation intake of chemical as an infant (1.45×10^{-3} µg/m^3)
$EC_{(child)}$	=	direct inhalation intake of chemical as a child (1.45×10^{-3} µg/m^3)
$EC_{(adult)}$	=	direct inhalation intake of chemical as an adult (0 µg/m^3)
RfC	=	inhalation reference concentration (1.00×10^{-1} mg/m^3)
1,000	=	conversion factor (µg/mg)

$$HQ_D = \frac{\frac{1}{5} \cdot 1.45 \cdot 10^{-3} + \frac{4}{5} \cdot 1.45 \cdot 10^{-3}}{(1.00 \cdot 10^{-1} \cdot 1{,}000)} = 1.45 \cdot 10^{-5}$$

Noncarcinogenic hazard from indirect exposure to vinyl chloride was calculated using Equation D-64.

$$HQ_I = \frac{\frac{1}{30} I_{indirect(infant)} + \frac{5}{30} I_{indirect(child)} + \frac{24}{30} \cdot I_{indirect(adult)}}{RfD} \qquad \text{Eq. D-64}$$

where

HQ_I	=	HQ for indirect exposures (dimensionless)
$I_{indirect(infant)}$	=	total indirect exposure as an infant (1.23 x 10^{-7} mg/kg of body weight-day)
$I_{indirect(child)}$	=	total indirect exposure as a child (1.87 x 10^{-7} mg/kg of body weight-day)
$I_{indirect(adult)}$	=	total indirect exposure as an adult (9.02 x 10^{-8} mg/kg of body weight-day)
RfD	=	oral reference dose (3.00 x 10^{-3} mg/kg of body weight-day)

$$HQ_I = \frac{\frac{1}{30} 1.23 \cdot 10^{-7} + \frac{5}{30} 1.87 \cdot 10^{-7} + \frac{24}{30} \cdot 9.02 \cdot 10^{-8}}{3.00 \cdot 10^{-3}} = 3.58 \cdot 10^{-5}$$

HQs were calculated to represent the noncarcinogenic hazard associated with vinyl chloride and a particular exposure pathway. A total HQ is then calculated by estimating total noncarcinogenic hazard from all exposure pathways associated with a particular human receptor. Because this example is for only vinyl chloride, the HQs for the direct and indirect pathways are equal to the HIs for the direct and indirect pathways, respectively. Therefore, the total non-cancer HQ (HQ_T) from all exposure pathways for a particular chemical, both direct and indirect, was calculated as the sum of the HIs (i.e., HQs) for vinyl chloride using equation D-67.

$$HQ_T = HQ_D + HQ_I \qquad \text{Eq. D-67}$$

where

HQ_T	=	total HQ from vinyl chloride (dimensionless)
HQ_D	=	HQ from direct inhalation exposure to vinyl chloride (1.45 x 10^{-5})
HQ_I	=	HQ from indirect exposures to vinyl chloride (3.58 x 10^{-5})

$$HQ_T = 1.45 \cdot 10^{-5} + 3.58 \cdot 10^{-5} = 5.03 \cdot 10^{-5}$$

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