

Appendix D

Air Modeling Results

Appendix D1

Outdoor Air Exposure Point Calculations For OU4

APPENDIX D1

CALCULATION OF OUTDOOR AIR CONCENTRATIONS

General

Outdoor air concentrations of the COPCs could result from volatilization of constituents in the groundwater or soil. To evaluate potential risks associated with outdoor air, it is necessary to estimate exposure point concentrations (EPCs) associated with each component. The final outdoor air concentrations used in the exposure and risk calculations were based on the highest predicted concentration selected from either the predicted outdoor vapors from groundwater, or the predicted outdoor vapors from soil.

Outdoor Vapors From Groundwater

In this case, outdoor vapors originate from dissolved chemicals in groundwater located some distance below the ground surface. The relationship between outdoor air and dissolved groundwater is represented by the volatilization factor (VF). The calculation of VF is based on several assumptions:

- a constant concentration of the chemical in groundwater
- linear equilibrium partitioning between dissolved chemicals in groundwater and chemical vapors at the groundwater table
- steady state vapor- and liquid-phase diffusion through the capillary fringe and vadose zones to the ground surface
- no loss of chemical as it diffuses upward toward the ground surface
- steady state well mixed atmospheric dispersion of the emanating vapors within the breathing zone as modeled by a “box model” for air dispersion

The VF for outdoor vapors from groundwater is calculated using the following equations (ASTM, 2004):

$$VF = H \times 1000 / [1 + ((100 \times U_m \times d_a \times L_{GW}) / (W_{ga} \times D_{ws}^{eff}))]$$

and

$$D_{ws}^{eff} = (h_{cap} + h_v) \times [(h_{cap} / D_{cap}^{eff}) + (h_v / D_s^{eff})]^{-1}$$

and

$$D_{cap}^{eff} = D_a \times (\theta_{acapp}^{3.33} / \theta_T^2) + D_w \times 1/H \times (\theta_{wcapp}^{3.33} / \theta_T^2)$$

and

$$D_s^{eff} = D_a \times (\theta_{as}^{3.33} / \theta_T^2) + D_w \times 1/H \times (\theta_{ws}^{3.33} / \theta_T^2)$$

Where:

- VF = volatilization factor from groundwater to outdoor air (mg/m³ – air / mg/L – water)
- H = vadose zone chemical specific Henry's Law constant (L-water / L-air)
- U_m = mean annual wind speed (m/s)
- d_a = breathing zone height (cm)
- L_{GW} = depth to groundwater (cm)
- W_{ga} = dimension of soil source area parallel to wind direction (cm)
- D_{ws}^{eff} = effective diffusion coefficient between groundwater and soil (cm²/s)
- h_{cap} = thickness of capillary fringe (cm)
- h_v = thickness of vadose zone (cm)
- D_{cap}^{eff} = effective diffusion coefficient for the capillary fringe (cm²/s)
- D_s^{eff} = effective diffusion coefficient in soil based on vapor-phase concentration (cm²/s)
- D_a = chemical-specific diffusion coefficient in air (cm²/s)
- θ_{acapp} = volumetric air content in capillary fringe soils (cm³-air/cm³-soil)
- θ_T = total soil porosity (cm³/cm³-soil)
- D_w = chemical-specific diffusion coefficient in water (cm²/s)
- θ_{wcap} = volumetric water content in capillary fringe soils (cm³-water/cm³-soil)
- θ_{as} = volumetric air content in vadose zone soils (cm³-air/cm³-soil)
- θ_{ws} = volumetric water content in vadose zone soils (cm³-water/cm³-soil)

VFs were calculated using site-specific, and chemical-specific default values for the input variables as presented in Table D-1. The results are presented in Table D-1. These VFs were applied to the groundwater exposure point concentrations (EPCs) to calculate corresponding EPCs for outdoor air. The results of these calculations are presented in Table D-1.

Outdoor Vapors From Soil

In this case, outdoor vapors originate from chemicals in subsurface soil. The relationship between outdoor air and subsurface soil is represented by a volatilization factor (VF). The equations used to calculate VF are different for residential, commercial/industrial and construction scenarios as discussed in the subsections below. In the event that the time-averaged flux exceeds that which would occur if all the chemical initially present in the soil volatilized during the exposure period, then the volatilization factor can be determined from a mass balance approach assuming that all chemical present in the subsurface soil layer volatilizes during the exposure period. The equations for the volatilization factors and the mass balance approach are from the EPA Soil Screening Guidance (EPA, 1996) and the EPA Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (EPA, 2002):

Total soil was used to predict outdoor vapors for the future residential scenario as well as for the current/future industrial worker and construction worker. In this case, outdoor vapors originate from chemicals in soil located some distance below the ground surface. The relationship between outdoor air and subsurface soil is represented by the volatilization factor (VF). The calculation of VF is based on several assumptions:

- A constant chemical concentration in subsurface soils
- Linear equilibrium partitioning within the soil matrix between sorbed, dissolved and vapor phases, where the partitioning is a function of constant chemical- and soil- specific parameters
- Steady-state vapor- and liquid- phase diffusion through the vadose zone to the ground surface

- No loss of chemical as it diffuses toward ground surface (i.e., no biodegradation)
- Steady well-mixed atmospheric dispersion of the emanating vapors within the breathing zone as modeled by a “box model” for air dispersion

The VF for outdoor vapors from soil is calculated using slightly different equations for residential, industrial/commercial and construction worker scenarios.

Outdoor Vapors from Soil – Residential Scenario

The soil-to-air VF is used to define the relationship between the concentration of the contaminant in soil and the flux of the volatilized contaminant to air. The residential scenario VF for outdoor vapors from soil is calculated using the following equations from the EPA Soil Screening Guidance (EPA, 1996):

$$VF = [Q/C \times 0.0001 \times (3.14 \times D_A \times t)^{1/2} / (2 \times r_s \times D_A)]$$

and

$$D_A = [(\theta_{as}^{3.33} \times D_a \times H + \theta_{ws}^{3.33} \times D_w) / \theta_T^2] / (r_s \times K_{sv} + \theta_{ws} + \theta_{as} \times H)$$

Where:

- VF = volatilization factor from soil to outdoor air (m³/kg)
 Q/C = inverse of the mean concentration at the center of square source (g/m²-s / kg/m³)
 D_A = apparent diffusivity (cm²/s)
 t = exposure interval for vapor flux (s)
 r_s = vadose zone dry bulk density of soil (g-soil/cm³-soil)
 θ_{as} = air-filled soil porosity (cm³-air/cm³-soil)
 D_a = chemical-specific diffusion coefficient in air (cm²/s)
 H = vadose zone chemical specific Henry’s Law constant (L-water / L-air)
 θ_{ws} = water-filled soil porosity (cm³-water/cm³-soil)
 D_w = chemical-specific diffusion coefficient in water (cm²/s)
 θ_T = total soil porosity (cm³/cm³-soil)
 K_{sv} = chemical-specific soil-water partition coefficient (cm³-water/g-soil)

VFs were calculated using site-specific, chemical-specific default values for the input variables as presented in Table D-2. The results are presented in Table D-2. These VFs were applied to the total soil exposure point concentrations (EPCs) to calculate

corresponding EPCs for outdoor air. The results of these calculations are presented in Table D-2.

Outdoor Vapors from Soil – Commercial/Industrial Scenario

The soil-to-air VF is used to define the relationship between the concentration of the contaminant in soil and the flux of the volatilized contaminant to air. The commercial/industrial scenario VF for outdoor vapors from soil is calculated using the following equations from the EPA Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (EPA, 2002):

$$VF = [Q/C_{vol} \times 0.0001 \times (3.14 \times D_A \times t)^{1/2} / (2 \times r_s \times D_A)]$$

and

$$D_A = [(\theta_{as}^{3.33} \times D_a \times H + \theta_{ws}^{3.33} \times D_w) / \theta_T^2] / (r_s \times K_{sv} + \theta_{ws} + \theta_{as} \times H)$$

and

$$Q/C_{vol} = A \times \exp [(\ln A_{site} - B)^2 / C]$$

Where:

- VF = volatilization factor from soil to outdoor air (m³/kg)
- Q/C_{vol} = inverse of the mean concentration at the center of square source (g/m²-s / kg/m³)
- D_A = apparent diffusivity (cm²/s)
- t = exposure interval for vapor flux (s)
- r_s = vadose zone dry bulk density of soil (g-soil/cm³-soil)
- θ_{as} = air-filled soil porosity (cm³-air/cm³-soil)
- D_a = chemical-specific diffusion coefficient in air (cm²/s)
- H = vadose zone chemical specific Henry’s Law constant (L-water / L-air)
- θ_{ws} = water-filled soil porosity (cm³-water/cm³-soil)
- D_w = chemical-specific diffusion coefficient in water (cm²/s)
- θ_T = total soil porosity (cm³/cm³-soil)
- K_{sv} = chemical-specific soil-water partition coefficient (cm³-water/g-soil)
- A_{site} = Areal extent of the site or contamination (0.5 acres)
- A = Dispersion constant (= 14.1901 for Zone 5 at Lincoln, NE)
- B = Dispersion constant (= 18.5634 for Zone 5 at Lincoln, NE)
- C = Dispersion constant (= 210.5281 for Zone 5 at Lincoln, NE)

VFs were calculated using site-specific, chemical-specific default values for the input variables as presented in Table D-3. The results are presented in Table D-3. These VFs

were applied to the total soil exposure point concentrations (EPCs) to calculate corresponding EPCs for outdoor air. The results of these calculations are presented in Table D-3.

Outdoor Vapors from Soil – Construction Worker Scenario

The soil-to-air VF is used to define the relationship between the concentration of the contaminant in soil and the flux of the volatilized contaminant to air. The construction worker scenario VF for outdoor vapors from soil is calculated using the following equations from the EPA Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (EPA, 2002):

$$VF = [Q/C_{sa} \times 1/F_D \times 0.0001 \times (3.14 \times D_A \times t)^{1/2} / (2 \times r_s \times D_A)]$$

and

$$D_A = [(\theta_{as}^{3.33} \times D_a \times H + \theta_{ws}^{3.33} \times D_w) / \theta_T^2] / (r_s \times K_{sv} + \theta_{ws} + \theta_{as} \times H)$$

and

$$Q/C_{sa} = A \times \exp [(\ln A_c - B)^2 / C]$$

Where:

- VF = volatilization factor from soil to outdoor air (m³/kg)
- Q/C_{sa} = inverse of the mean concentration at the center of square source (g/m²-s / kg/m³)
- F_D = dispersion correction factor (0.185)
- D_A = apparent diffusivity (cm²/s)
- t = exposure interval for vapor flux (s)
- r_s = vadose zone dry bulk density of soil (g-soil/cm³-soil)
- θ_{as} = air-filled soil porosity (cm³-air/cm³-soil)
- D_a = chemical-specific diffusion coefficient in air (cm²/s)
- H = vadose zone chemical specific Henry's Law constant (L-water / L-air)
- θ_{ws} = water-filled soil porosity (cm³-water/cm³-soil)
- D_w = chemical-specific diffusion coefficient in water (cm²/s)
- θ_T = total soil porosity (cm³/cm³-soil)
- K_{sv} = chemical-specific soil-water partition coefficient (cm³-water/g-soil)
- A_c = Areal extent of the site or contamination (0.5 acres)
- A = Dispersion constant (= 2.4538)
- B = Dispersion constant (= 17.566)
- C = Dispersion constant (= 189.0426)

VFs were calculated using site-specific, chemical-specific default values for the input variables as presented in Table D-4. The results are presented in Table D-4. These VFs were applied to the total soil exposure point concentrations (EPCs) to calculate corresponding EPCs for outdoor air. The results of these calculations are presented in Table D-4.

Outdoor Air Final

The final outdoor air concentrations used in the exposure and risk calculations were based on the highest predicted concentration selected from the predicted outdoor vapors from groundwater (Table D-1), or the predicted outdoor vapors from soil (Tables D-2 through D-4). The predicted values for groundwater and soil and final selection of outdoor air concentrations for each exposure scenario are summarized in Table D-5.

Table D-1 Calculation of Volatilization Factor for Groundwater to Outdoor Air

	$VF = H \times 1000 \times [1 / (1 + (100 \times U_m \times d_a \times L_{GW}) / (W_{ga} \times D_{ws}^{eff}))]$ $D_{ws}^{eff} = (h_{cap} + h_v) \times [(h_{cap} / D_{cap}^{eff}) + (h_v / D_s^{eff})]^{-1}$ $D_{cap}^{eff} = D_a \times (\theta_{acap}^{3.33} / \theta_T^2) + D_w \times (1/H) \times (\theta_{wcap}^{3.33} / \theta_T^2)$ $D_s^{eff} = D_a \times (\theta_{as}^{3.33} / \theta_T^2) + D_w \times (1/H) \times (\theta_{ws}^{3.33} / \theta_T^2)$																
H	Henry Law Constant																
U _m	Wind speed (m/s)																
d _a	Breathing Zone height (cm)																
L _{GW}	Average Depth to groundwater (cm)																
W _{ga}	dimension of soil source area parallel to wind direction (cm) used a 0.5 acre square source																
D _{ws} ^{eff}	effective diffusion coefficient between groundwater and soil (cm ² /s)																
h _{cap}	capillary fringe thickness (cm)																
h _v	Thickness of vadose zone (cm)																
D _{cap} ^{eff}	effective diffusion coefficient for the capillary fringe (cm ² /s)																
D _s ^{eff}	effective diffusion coefficient in soil based on vapor-phase concentration (cm ² /s)																
θ _{acap}	volumetric air content in capillary fringe soils (cm ³ -air/cm ³ -soil)																
θ _T	total soil porosity (cm ³ /cm ³ -soil)																
θ _{wcap}	volumetric water content in capillary fringe soils (cm ³ -water/cm ³ -soil)																
θ _{as}	volumetric air content in vadose zone soils (cm ³ -air/cm ³ -soil)																
θ _{ws}	volumetric water content in vadose zone soils (cm ³ -water/cm ³ -soil)																
COPC	H	Da	Dw	Um	d _a	Lgw (cm)	Wga (cm)	Deff(ws)	hcap (cm)	hv (cm)	Deff(cap)	Deff(s)	Theta acap	Theta wcap	Theta a	Theta w	Theta t
Acetone	1.59E-03	0.124	1.14E-05	4.69	200	1500	4498	8.18E-03	5	1495	1.77E-03	8.29E-03	0.044	0.4	0.27	0.17	0.44
cis-1,2-DCE	0.167	0.0736	1.13E-05	4.69	200	1500	4498	3.09E-03	5	1495	2.81E-05	4.86E-03	0.044	0.4	0.27	0.17	0.44
trans-1,2-DCE	0.385	0.0707	1.19E-05	4.69	200	1500	4498	2.55E-03	5	1495	1.86E-05	4.67E-03	0.044	0.4	0.27	0.17	0.44
1,2-DCE Total	0.167	0.0736	1.13E-05	4.69	200	1500	4498	3.09E-03	5	1495	2.81E-05	4.86E-03	0.044	0.4	0.27	0.17	0.44
PCE	0.754	0.072	8.20E-06	4.69	200	1500	4498	2.23E-03	5	1495	1.40E-05	4.75E-03	0.044	0.4	0.27	0.17	0.44
TCE	0.422	0.079	9.10E-06	4.69	200	1500	4498	2.63E-03	5	1495	1.77E-05	5.21E-03	0.044	0.4	0.27	0.17	0.44
VC	1.11	0.106	1.23E-06	4.69	200	1500	4498	2.94E-03	5	1495	1.69E-05	7.00E-03	0.044	0.4	0.27	0.17	0.44

Table D-1 Calculation of Volatilization Factor for Groundwater to Outdoor Air (cont.)

OUTDOOR AIR VAPORS FROM GROUNDWATER						
VF (mg/m3 air / mg/L water)	GW RME mg/L	RME Outdoor Air mg/m3	RME Outdoor Air ug/m3	GW CTE mg/L	CTE Outdoor Air mg/m3	CTE Outdoor Air ug/m3
4.16E-07	2.1	8.74E-07	8.74E-04	0.728	3.03E-07	3.03E-04
1.65E-05	1.71	2.82E-05	2.82E-02	0.309	5.09E-06	5.09E-03
3.14E-05	0.014	4.39E-07	4.39E-04	0.014	4.39E-07	4.39E-04
1.65E-05	1.56	2.57E-05	2.57E-02	0.273	4.50E-06	4.50E-03
5.37E-05	34.6	1.86E-03	1.86E+00	3.35	1.80E-04	1.80E-01
3.55E-05	1.8	6.39E-05	6.39E-02	0.323	1.15E-05	1.15E-02
1.04E-04	ND	NC	NC	ND	NC	NC

Table D-2 Calculation of Residential Scenario Volatilization Factor (Soil to Outdoor Air)

Chemical	Q/C	DA cm ² /s	T s	<i>pb</i> g/cm ³	VF (m ³ /kg)
PCE	81.64	0.002025952	9.50E+08	1.5	3302
TCE	81.64	0.00123761	9.50E+08	1.5	4225
VC	81.64	0.012188723	9.50E+08	1.5	1346

Chemical	Theta a	Di cm ² /s	H'	Theta w	Dw cm ² /s	n	<i>pb</i> g/cm ³	Kd cm ³ /g	Koc cm ³ /g	foc
PCE	0.27	0.072	0.754	0.17	8.20E-06	0.44	1.5	0.93	155	0.006
TCE	0.27	0.079	0.422	0.17	9.10E-06	0.44	1.5	0.996	166	0.006
VC	0.27	0.106	1.11	0.17	1.23E-06	0.44	1.5	0.1116	18.6	0.006

Table D-2 Calculation of Residential Scenario Volatilization Factor (Soil to Outdoor Air) cont.

Chemical	VF (m ³ /kg)	RME Soil mg/kg	RME Outdoor Air mg/m ³	RME Outdoor Air ug/m ³	CTE Soil mg/kg	CTE Outdoor Air mg/m ³	CTE Outdoor Air ug/m ³
PCE	3302	2550	7.72E-01	7.72E+02	444	1.34E-01	1.34E+02
TCE	4225	7.7	1.82E-03	1.82E+00	3.75	8.88E-04	8.88E-01
VC	1346	0.2	1.49E-04	1.49E-01	0.2	1.49E-04	1.49E-01

Table D-3 Calculation of Commercial/Industrial Scenario Volatilization Factor (Soil to Outdoor Air)

A =	14.1901									
B =	18.5634									
C =	210.5281									
Q/C _{vol} =	82.6									
Chemical	Q/C _{vol}	DA cm ² /s	T s	<i>pb</i> g/cm ³						
					VF (m ³ /kg)					
PCE	82.6	0.002026	9.50E+08	1.5	3341					
TCE	82.6	0.001238	9.50E+08	1.5	4274					
VC	82.6	0.012189	9.50E+08	1.5	1362					
Chemical	Theta a	Di cm ² /s	H'	Theta w	Dw cm ² /s	n	<i>pb</i> g/cm ³	Kd cm ³ /g	Koc cm ³ /g	foc
PCE	0.27	0.072	0.754	0.17	8.20E-06	0.44	1.5	0.93	155	0.006
TCE	0.27	0.079	0.422	0.17	9.10E-06	0.44	1.5	0.996	166	0.006
VC	0.27	0.106	1.11	0.17	1.23E-06	0.44	1.5	0.1116	18.6	0.006

Table D-3 Calculation of Commercial/Industrial Scenario Volatilization Factor (Soil to Outdoor Air) cont.

Chemical	VF (m ³ /kg)	RME Soil mg/kg	RME Outdoor Air mg/m ³	RME Outdoor Air ug/m ³	CTE Soil mg/kg	CTE Outdoor Air mg/m ³	CTE Outdoor Air ug/m ³
PCE	3341	2550	7.63E-01	7.63E+02	444	1.33E-01	1.33E+02
TCE	4274	7.7	1.80E-03	1.80E+00	3.75	8.77E-04	8.77E-01
VC	1362	0.2	1.47E-04	1.47E-01	0.2	1.47E-04	1.47E-01

Table D-4 Calculation of Construction Worker Scenario Volatilization Factor (Soil to Outdoor Air)

Q/C _{sa}	14.31									
Chemical	Q/C _{sa}	DA cm ² /s	T s	<i>pb</i> g/cm ³	F _D	VF (m ³ /kg)				
PCE	14.3	0.002026	1.04E+07	1.5	0.185	327				
TCE	14.3	0.001238	1.04E+07	1.5	0.185	418				
VC	14.3	0.012189	1.04E+07	1.5	0.185	133				
Chemical	Theta a	Di cm ² /s	H'	Theta w	Dw cm ² /s	n	<i>pb</i> g/cm ³	Kd cm ³ /g	Koc cm ³ /g	foc
PCE	0.27	0.072	0.754	0.17	8.20E-06	0.44	1.5	0.93	155	0.006
TCE	0.27	0.079	0.422	0.17	9.10E-06	0.44	1.5	0.996	166	0.006
VC	0.27	0.106	1.11	0.17	1.23E-06	0.44	1.5	0.1116	18.6	0.006

Table D-4 Calculation of Construction Worker Scenario Volatilization Factor (Soil to Outdoor Air) cont.

Chemical	VF (m ³ /kg)	RME Soil mg/kg	RME Outdoor Air mg/m ³	RME Outdoor Air ug/m ³	CTE Soil mg/kg	CTE Outdoor Air mg/m ³	CTE Outdoor Air ug/m ³
PCE	327	2550	7.80E+00	7.80E+03	444	1.36E+00	1.36E+03
TCE	418	7.7	1.84E-02	1.84E+01	3.75	8.97E-03	8.97E+00
VC	133	0.2	1.50E-03	1.50E+00	0.2	1.50E-03	1.50E+00

Table D-5 Final Outdoor Air Exposure Point Concentrations (Residential)

COPC	RME Groundwater mg/L	RME Soil mg/kg	RME Outdoor Air From GW ug/m ³	Total Soil RME Outdoor Air From Soil ug/m ³	Selected RME Outdoor Air ug/m ³
Acetone	2.1	ND	8.74E-04	NC	8.74E-04
cis-1,2-Dichloroethene	1.71	ND	2.82E-02	NC	2.82E-02
trans-1,2-Dichloroethene	14	ND	4.39E-04	NC	4.39E-04
Tetrachloroethene	34.6	2550	1.86	7.72E+02	7.72E+02
Trichloroethene	1.8	7.7	6.39E-02	1.82E+00	1.82E+00
Vinyl Chloride	ND	0.2	NC	1.49E-01	1.49E-01

COPC	CTE Groundwater mg/L	CTE Soil mg/kg	CTE Outdoor Air From GW ug/m ³	Total Soil CTE Outdoor Air From Soil ug/m ³	Selected CTE Outdoor Air ug/m ³
Acetone	0.728	ND	3.03E-04	NC	3.03E-04
cis-1,2-Dichloroethene	0.309	ND	5.09E-03	NC	5.09E-03
trans-1,2-Dichloroethene	14	ND	4.39E-04	NC	4.39E-04
Tetrachloroethene	3.35	444	1.80E-01	1.34E+02	1.34E+02
Trichloroethene	0.323	3.75	1.15E-02	8.88E-01	8.88E-01
Vinyl Chloride	ND	0.2	NC	1.49E-01	1.49E-01

Table D-5 Final Outdoor Air Exposure Point Concentrations (Industrial/Commercial)

COPC	RME Groundwater mg/L	RME Soil mg/kg	RME Outdoor Air From GW ug/m ³	Total Soil RME Outdoor Air From Soil ug/m ³	Selected RME Outdoor Air ug/m ³
Acetone	2.1	ND	8.74E-04	NC	8.74E-04
cis-1,2-Dichloroethene	1.71	ND	2.82E-02	NC	2.82E-02
trans-1,2-Dichloroethene	14	ND	4.39E-04	NC	4.39E-04
Tetrachloroethene	34.6	2550	1.86	7.63E+02	7.63E+02
Trichloroethene	1.8	7.7	6.39E-02	1.80E+00	1.80E+00
Vinyl Chloride	ND	0.2	NC	1.47E-01	1.47E-01

COPC	CTE Groundwater mg/L	CTE Soil mg/kg	CTE Outdoor Air From GW ug/m ³	Total Soil CTE Outdoor Air From Soil ug/m ³	Selected CTE Outdoor Air ug/m ³
Acetone	0.728	ND	3.03E-04	NC	3.03E-04
cis-1,2-Dichloroethene	0.309	ND	5.09E-03	NC	5.09E-03
trans-1,2-Dichloroethene	14	ND	4.39E-04	NC	4.39E-04
Tetrachloroethene	3.35	444	1.80E-01	1.33E+02	1.33E+02
Trichloroethene	0.323	3.75	1.15E-02	8.77E-01	8.77E-01
Vinyl Chloride	ND	0.2	NC	1.47E-01	1.47E-01

Table D-5 Final Outdoor Air Exposure Point Concentrations (Construction Worker)

COPC	RME Groundwater mg/L	RME Soil mg/kg	RME Outdoor Air From GW ug/m ³	Total Soil RME Outdoor Air From Soil ug/m ³	Selected RME Outdoor Air ug/m ³
Acetone	2.1	ND	8.74E-04	NC	8.74E-04
cis-1,2-Dichloroethene	1.71	ND	2.82E-02	NC	2.82E-02
trans-1,2-Dichloroethene	14	ND	4.39E-04	NC	4.39E-04
Tetrachloroethene	34.6	2550	1.86	7.80E+03	7.80E+03
Trichloroethene	1.8	7.7	6.39E-02	1.84E+01	1.84E+01
Vinyl Chloride	ND	0.2	NC	1.50E+00	1.50E+00

COPC	CTE Groundwater mg/L	CTE Soil mg/kg	CTE Outdoor Air From GW ug/m ³	Total Soil CTE Outdoor Air From Soil ug/m ³	Selected CTE Outdoor Air ug/m ³
Acetone	0.728	ND	3.03E-04	NC	3.03E-04
cis-1,2-Dichloroethene	0.309	ND	5.09E-03	NC	5.09E-03
trans-1,2-Dichloroethene	14	ND	4.39E-04	NC	4.39E-04
Tetrachloroethene	3.35	444	1.80E-01	1.36E+03	1.36E+03
Trichloroethene	0.323	3.75	1.15E-02	8.97E+00	8.97E+00
Vinyl Chloride	ND	0.2	NC	1.50E+00	1.50E+00

Appendix D2

Calculation of Sewer Water Vapors and Vapors From Groundwater in an Open Excavation

APPENDIX D2

CALCULATION OF SEWER WATER VAPORS AND VAPORS FROM GROUNDWATER IN AN OPEN EXCAVATION

General

There are no well-established models available for estimating volatilization of volatile organic chemicals from sanitary sewer water or ground water into a construction/utility trench. To estimate air concentrations of volatile chemicals in a trench, the volatilization of gases from sewer water and groundwater were estimated using mass transfer and diffusion coefficients and a box model to estimate dispersion of the contaminants in the air inside the trench. To estimate the exposure point concentration for air in the trench, two different methods were used to estimate the volatilization into the trench. The highest predicted concentration from the two methods was selected as the final exposure point concentration for the construction worker performing work in the trench.

Method 1 Volatilization of Contaminants from Sanitary Sewer Water

In this case, a construction worker was assumed to perform work on the sanitary sewer and could be exposed to vapors volatilizing from the sewer water. The model used to assess exposure to construction workers from vapors emitted from pooled sewer water is based on an approach developed from the USEPA Superfund Exposure Assessment Manual (USEPA, 1988). This model assumes a steady-state presence of volatile organic chemicals (the supply of VOCs is constantly renewed and does not diminish over time). In addition, it is assumed that the air is uniformly mixed throughout the breathing zone. The volatilization factor (VF) for vapors from sewer water was calculated from the following equations:

$$VF = (K_i \times A \times F \times 10^{-3} \times 10^4 \times 3600) / (ACH \times V)$$

$$K_i = 1 / [(1/k_{iL}) + (RT/H_i \times K_{iG})]$$

$$k_{iL} = (MW_{O_2}/MW_i)^{0.5} \times (T/298) \times k_{L,O_2}$$

and

$$k_{iG} = (MW_{H_2O}/MW_i)^{0.335} \times (T/298)^{1.005} \times k_{G,H_2O}$$

Where:

K_i	= overall mass transfer coefficient of contaminant (cm/s)
A	= area of the trench (m ²)
F	= fraction of floor through which contaminant can enter (unitless) 100%
ACH	= air changes per hour (2 h ⁻¹)
V	= volume of trench (m ³)
10 ⁻³	= conversion factor L/cm ³
10 ⁴	= conversion factor cm ² /m ²
3600	= conversion factor s/hr
k_{iL}	= liquid-phase mass transfer coefficient of i (cm/s)
R	= ideal gas constant (8.2E-05 atm·m ³ /mole·°K)
T	= average system absolute temperature (299 °K)
H_i	= Henry's Law constant (atm·m ³ /mole)
k_{iG}	= gas-phase mass transfer coefficient of i (cm/s)
MW_{O_2}	= molecular weight of O ₂ (32 g/mole)
MW_i	= molecular weight of i (g/mole)
k_{L,O_2}	= liquid-phase mass transfer coefficient of oxygen at 25 °C (0.002 cm/s)
MW_{H_2O}	= molecular weight of water (18 g/mole)
k_{G,H_2O}	= gas-phase mass transfer coefficient of water vapor at 25 °C (0.833 cm/s)

For purposes of this evaluation, it was assumed that an excavation trench intercepting a sewer line would measure approximately 8 feet long (2.44 meters), 3 feet wide (0.91 meters) and 8 feet deep (2.44 meters). VFs were calculated using the chemical-specific values for Molecular Weight and Henry's Law Constants as presented in Tables D-6 and D-7. The results of the calculations are also presented in Tables D-6 and D-7. These VFs

were then applied to the sewer water exposure point concentrations (EPCs) to calculate corresponding EPCs for vapors in the trench. The results of these calculations are also presented in Table D-6 and D-7 for the RME and CTE scenarios.

Method 2 Volatilization of Contaminants from Groundwater

In this case, a construction worker was assumed to perform work in the trench and could be exposed to vapors volatilizing from groundwater. The model used to assess exposure to construction workers from vapors emitted from groundwater is based on an approach developed from the USEPA Superfund Exposure Assessment Manual (USEPA, 1988). This model assumes a steady-state presence of volatile organic chemicals (the supply of VOCs is constantly renewed and does not diminish over time). In addition, it is assumed that the air is uniformly mixed throughout the breathing zone. The volatilization factor (VF) for vapors from groundwater was calculated from the following equations:

$$VF = (H_i \times D_{air} \times AC_{vad}^{3.33} \times A \times F \times 10^{-3} \times 10^4 \times 3600) / (R \times T \times L_d \times ACH \times V \times Por_{vad}^2)$$

$$L_d = L_{gw} - D_{trench}$$

Where:

H_i	= Henry's Law constant (atm·m ³ /mole)
D_{air}	= diffusion coefficient in air (cm ² /s)
AC_{vad}	= volumetric air content in vadose zone soil (0.27 cm ³ /cm ³)
A	= area of the trench (m ²)
F	= fraction of floor through which contaminant can enter (unitless) 100%
R	= ideal gas constant (8.2E-05 atm·m ³ /mole·°K)
T	= average system absolute temperature (299 °K)
L_d	= distance between trench bottom and groundwater (cm)
L_{gw}	= depth to groundwater (cm)
D_{trench}	= depth of trench (cm)
ACH	= air changes per hour (2 h ⁻¹)
V	= volume of trench (m ³)
Por_{vad}	= total soil porosity in vadose zone (0.44 cm ³ /cm ³)
10^{-3}	= conversion factor L/cm ³
10^4	= conversion factor cm ² /m ²
3600	= conversion factor s/hr

For purposes of this evaluation, it was assumed that an excavation trench intercepting a sewer line would measure approximately 8 feet long (2.44 meters), 3 feet wide (0.91 meters) and 8 feet deep (2.44 meters). VFs were calculated using the chemical-specific values for Henry's Law Constants and D_{air} as presented in Tables D-8 and D-9. The results are also presented in Tables D-8 and D-9. These VFs were applied to the groundwater exposure point concentrations (EPCs) to calculate corresponding EPCs for vapors in the trench. The results of these calculations are also presented in Tables D-8 and D-9 for the RME and CTE scenarios.

Table D-6
Inhalation RME Exposure Point Concentrations For Construction/Utility Workers In A Sewer Trench
Due To Volatiliation From Sewer Water
Riverfront OU4

RME Exposure-point concentrations (inhalation) for construction/utility workers in a sewer trench:	CAS No.	Molecular Weight MWi g/mol	Henry's Law Constant Hi atm-m3/mol	Gas-Phase Mass Transfer Coefficient KiG cm/s	Liquid-Phase Mass Transfer Coefficient KiL cm/s	Overall Mass Transfer Coefficient Ki cm/s	Concentration of Contaminant in Groundwater Cgw ug/L	Volatilization Factor VF L/m3	Concentration of Contaminant in Trench Ctrench ug/m3	Concentration of Contaminant in Trench Ctrench mg/m3
Volatile Organic Compounds (VOCs)										
Bromomethane	74-83-9	94.94	6.34E-03	4.79E-01	1.17E-03	1.15E-03	2.20E+00	8.52E+00	1.87E+01	1.87E-02
Chloroform	67-66-3	119.38	3.71E-03	4.43E-01	1.04E-03	1.02E-03	6.01E+00	7.55E+00	4.54E+01	4.54E-02
Tetrachloroethene	127-18-4	165.83	1.84E-02	3.97E-01	8.82E-04	8.79E-04	3.00E+00	6.49E+00	1.95E+01	1.95E-02

Table D-7
Inhalation CTE Exposure Point Concentrations For Construction/Utility Workers In A Sewer Trench
Due To Volatilization From Sewer Water
Riverfront OU4

CTE Exposure-point concentrations (inhalation) for construction/utility workers in a sewer trench:	CAS No.	Molecular Weight MWi g/mol	Henry's Law Constant Hi atm-m ³ /mol	Gas-Phase Mass Transfer Coefficient KiG cm/s	Liquid-Phase Mass Transfer Coefficient KiL cm/s	Overall Mass Transfer Coefficient Ki cm/s	Concentration of Contaminant in Groundwater Cgw ug/L	Volatilization Factor VF L/m ³	Concentration of Contaminant in Trench Ctrench ug/m ³	Concentration of Contaminant in Trench Ctrench mg/m ³
Volatile Organic Compounds (VOCs)										
Bromomethane	74-83-9	94.94	6.34E-03	4.79E-01	1.17E-03	1.15E-03	1.70E+00	8.52E+00	1.45E+01	1.45E-02
Chloroform	67-66-3	119.38	3.71E-03	4.43E-01	1.04E-03	1.02E-03	2.09E+00	7.55E+00	1.58E+01	1.58E-02
Tetrachloroethene	127-18-4	165.83	1.84E-02	3.97E-01	8.82E-04	8.79E-04	1.98E+00	6.49E+00	1.28E+01	1.28E-02

Table D-8
Inhalation RME Exposure Point Concentrations For Construction/Utility Workers In A Sewer Trench
Due To Volatilization From Groundwater
Riverfront OU4

RME Exposure-point concentrations (inhalation) for construction/utility workers in a trench: Vapors from Groundwater	CAS No.	Molecular Weight MWi g/mol	Henry's Law Constant Hi atm-m3/mol	Diffusion Coefficient in Air Dair cm2/s	Concentration of Contaminant in Groundwater Cgw ug/L	Volatilization Factor VF L/m3	Concentration of Contaminant in Trench Ctrench ug/m3	Concentration of Contaminant in Trench Ctrench mg/m3
Volatile Organic Compounds (VOCs)								
Acetone	67-64-1	58.08	3.88E-05	1.24E-01	2.10E+03	7.44E-05	1.56E-01	1.56E-04
1,2-Dichloroethene (total)	540-59-0	96.94	4.07E-03	7.36E-02	1.56E+03	4.63E-03	7.22E+00	7.22E-03
cis-1,2-Dichloroethene	156-59-2	96.94	4.07E-03	7.36E-02	1.71E+03	4.63E-03	7.92E+00	7.92E-03
trans-1,2-Dichloroethene	156-60-5	96.94	9.39E-03	7.07E-02	1.40E+01	1.03E-02	1.44E-01	1.44E-04
Tetrachloroethene	127-18-4	165.83	1.84E-02	7.20E-02	3.46E+04	2.05E-02	7.08E+02	7.08E-01
Trichloroethene	79-01-6	131.39	1.03E-02	7.90E-02	1.80E+03	1.26E-02	2.26E+01	2.26E-02

Table D-9
Inhalation CTE Exposure Point Concentrations For Construction/Utility Workers In A Sewer Trench
Due To Volatilization From Groundwater
Riverfront OU4

CTE Exposure-point concentrations (inhalation) for construction/utility workers in a trench: Vapors from Groundwater	CAS No.	Molecular Weight MWi g/mol	Henry's Law Constant Hi atm-m3/mol	Diffusion Coefficient in Air Dair cm2/s	Concentration of Contaminant in Groundwater Cgw ug/L	Volatilization Factor VF L/m3	Concentration of Contaminant in Trench Ctrench ug/m3	Concentration of Contaminant in Trench Ctrench mq/m3
Volatile Organic Compounds (VOCs)								
Acetone	67-64-1	58.08	3.88E-05	1.24E-01	7.28E+02	7.44E-05	5.41E-02	5.41E-05
1,2-Dichloroethene (total)	540-59-0	96.94	4.07E-03	7.36E-02	2.73E+02	4.63E-03	1.26E+00	1.26E-03
cis-1,2-Dichloroethene	156-59-2	96.94	4.07E-03	7.36E-02	3.09E+02	4.63E-03	1.43E+00	1.43E-03
trans-1,2-Dichloroethene	156-60-5	96.94	9.39E-03	7.07E-02	1.40E+01	1.03E-02	1.44E-01	1.44E-04
Tetrachloroethene	127-18-4	165.83	1.84E-02	7.20E-02	3.35E+03	2.05E-02	6.86E+01	6.86E-02
Trichloroethene	79-01-6	131.39	1.03E-02	7.90E-02	3.23E+02	1.26E-02	4.06E+00	4.06E-03