APPENDIX 3
DERIVATION OF RISK-BASED SCREENING LEVELS (RBSLs)

1.0 Conversion Calculations for Henry's Law Constants

Henry's Law constants ("H") are required to complete the calculation of risk-based screening levels (RBSLs) as provided below. The value H is a sensitive parameter in modeling volatilization, since it can vary with temperature, pressure, and concentration. The best value for H in any given model is obtained by direct measurement under field conditions. For the South Shore Remediation project, H was not previously measured, so literature values were obtained for use in the screening assessment. The highest calculated values of H (shown in bold text) were used to derive the RBSLs.

Chemical	Units	H	Conversion Factor	Converted H (unitless)
Benzene	atm	230	7.38E-04	0.17
	atm-m3/mole	5.50E-03	41.0	**0.23**
PCE	atm	1035	7.38E-04	**0.76**
	atm-m3/mole	na	41.0	na
TCE	atm	544	7.38E-04	**0.40**
	atm-m3/mole	8.92E-03	41.0	0.37
1,2-DCA	atm	51	7.38E-04	0.04
	atm-m3/mole	1.10E-03	41.0	**0.05**
1,1-DCE	atm	1841	7.38E-04	**1.36**
	atm-m3/mole	1.50E-02	41.0	0.61
Chloroform	atm	171	7.38E-04	0.13
	atm-m3/mole	3.39E-03	41.0	**0.14**
1,1,2-TCA	atm	41	7.38E-04	0.03
	atm-m3/mole	1.18E-03	41.0	**0.05**
Bromoform	atm	35	7.38E-04	0.03
	atm-m3/mole	5.32E-04	41.0	0.02

References:
(1) ASTM. 1995. Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites. American Society for Testing and Materials.
(2) CalTOX. 1995.
(3) Nyer, E.K. 1993. Practical Techniques for Groundwater and Soil Remediation. Lewis Publishers. p. 36.

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2.0 Derivation of RBSLs

The following tables provide the values used to derive RBSLs at the risk management threshold of 1×10^{-5}. The equations used to complete the calculations are provided below.

Step 1: Calculate RBSL for inhalation of chemical vapors in air

From Table X2.2, Medium: Air

$$RBSL_{air}\left[\frac{\mu g}{m^3 - air}\right] = \frac{TR \times BW \times AT_c \times 365\frac{days}{years} \times 10^3\frac{\mu g}{mg}}{SF_i \times IR_{air} \times EF \times ED}$$

Where:
- $RBSL_{air}$ = risk-based screening level for inhalation of vapors
- TR = target excess individual lifetime cancer risk (unitless)
- BW = adult body weight (kg)
- AT_c = averaging time for carcinogens (years)
- SF_i = inhalation cancer slope factor $(mg/kg\text{-}day)^{-1}$
- IR_{air} = daily outdoor inhalation rate (m^3/day)
- EF = exposure frequency (days/years)
- ED = exposure duration (years)

Using the equation provided above and the values provided in the following spreadsheets gives the RBSL for inhalation.

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Step 2: Calculate RBSL for groundwater, assuming volatilization and transport of constituents through the vadose zone and emission at the ground surface followed by inhalation of chemical vapors from air

From Table X2.2, Medium: Groundwater, ambient (outdoor) vapor inhalation

$$RBSL_w\left[\frac{mg}{L-H_2O}\right]=\frac{RBSL_{air}\left[\frac{\mu g}{m^3-air}\right]}{VF_{wamb}}\times\times 10^3\,\frac{\mu g}{mg}$$

Where:
- $RBSL_w$ = risk-based screening level for inhalation of vapors that have migrated from the groundwater through the vadose zone to the soil surface and into the air
- $RBSL_{air}$ = given in Step 1 above
- VF_{wamb} = the cross-media volatilization factor from groundwater to ambient (outdoor) vapors (defined in Step 3, below)

Using this equation with gives the value in the box in the spreadsheet. This is the value of interest in this risk assessment.

Calculate VF_{wamb}

From Table X2.5:

$$VF_{wamb}\left[\frac{(mg/m^3-air)}{(mg/L-H_2O)}\right]=\frac{H}{1+\left[\frac{U_{air}\delta_{air}L_{GW}}{WD_{ws}^{eff}}\right]}\times 10^3\,\frac{L}{m^3}$$

Where:
- VF_{wamb} = the cross-media volatilization factor from groundwater to ambient (outdoor) vapors
- H = Henry's law constant [(cm^3-H_2O/cm^3-air)]
- U_{air} = wind speed above ground surface in ambient mixing zone (cm/s)
- d_{air} = ambient mixing zone height (cm)
- L_{GW} = depth to groundwater = h_{cap} + h_v (cm)
- W = Width of source area parallel to wind, or ground water flow direction (cm)
- D_{ws}^{eff} = effective diffusion coefficient between groundwater and soil surface (cm^2/s). See below.

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Calculate D_{ws}^{eff}

$$D_{ws}^{eff}\left[\frac{cm^2}{s}\right] = \left(h_{cap} + h_v\right)\left[\frac{h_{cap}}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}}\right]^{-1}$$

Where:

D_{ws}^{eff} = effective diffusion coefficient between groundwater and soil surface (cm^2/s)

h_{cap} = thickness of the capillary fringe (cm)

h_v = thickness of the vadose zone (cm)

D_{cap}^{eff} = effective diffusion through the capillary fringe (cm^2/s). See below.

D_s^{eff} = effective diffusion in soil based on vapor-phase concentration (cm^2/s). See below.

Calculate D_{cap}^{eff}

$$D_{cap}^{eff}\left[\frac{cm^2}{s}\right] = D^{air}\frac{\theta_{acap}^{3.33}}{\theta_T^2} + D^{wat}\frac{1}{H}\frac{\theta_{wcap}^{3.33}}{\theta_T^2}$$

Where:

D_{cap}^{eff} = effective diffusion through the capillary fringe (cm^2/s)

D^{air} = diffusion coefficient in air (cm^2/s)

D^{wat} = diffusion coefficient in water (cm^2/s)

θ_{acap} = volumetric air content in capillary fringe soils [(cm^3-air/cm^3-soil)]

θ_{wcap} = volumetric water content in capillary fringe soils [(cm^3-H_2O/cm^3-soil)]

θ_T = total soil porosity [(cm^3/cm^3-soil)]

H = Henry's law constant [(cm^3-H_2O/cm^3-air)]

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Calculate D_s^{eff}

$$D_s^{eff}\left[\frac{cm^2}{s}\right] = D^{air}\frac{\theta_{as}^{3.33}}{\theta_T^2} + D^{wat}\frac{1}{H}\frac{\theta_{ws}^{3.33}}{\theta_T^2}$$

Where:

D_s^{eff} = effective diffusion through the capillary fringe (cm^2/s)
D^{air} = diffusion coefficient in air (cm^2/s)
D^{wat} = diffusion coefficient in water (cm^2/s)
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-H_2O/cm^3-soil)]
θ_T = total soil porosity [(cm^3/cm^3-soil)]
H = Henry's law constant [(cm^3-H_2O/cm^3-air)]

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$RBSL_i$, outdoor air, commercial land use										
Risk-Based Screening Level	$RBSL_{inh}$	$\mu g/m^3$-air	2.81E+00	Diffusion coefficient in air	D_{air}	cm^2/s	6.60E-01	Cross-media volatilization factor	V_{wamb}	5.10E-04
Target excess individual lifetime cancer risk	TR	unitless	1.00E-05	Diffusion coefficient in water	D_{wat}	cm^2/s	8.80E-05	Effective diffusion coefficient in soil based on vapor-phase concentration	D_s	5.15E-02
Adult body weight	BW	kg	70	Henry's Law constant	H	cm^3-H_2O/cm^3-air	0.76	Effective diffusion coefficient through capillary fringe	D_{cap}	1.08E-04
Averaging time for carcinogens	AT_c	years	70	Thickness of capillary fringe	h_{cap}	cm	5	Effective diffusion coefficient between groundwater and soil surface	D_{eff}	3.48E-03
Inhalation cancer slope factor	SF_I	$(mg/kg\text{-}day)^{-1}$	0.051	Thickness of vadose zone	h_v	cm	168	Risk-Based Screening Level, ambient air, inhalation, commercial exposure	$RBSL_{inh}$	2.81E+00
Inhalation rate	IR_{air}	m^3/day	20	Depth to groundwater	L_{gw}	cm	173	Risk-Based Screening Level, groundwater to ambient air, commercial exposure	$RBSL_{gw\text{-}inh}$	5.50E+00
Exposure frequency	EF	days/year	250	Wind speed above ground surface in ambient mixing zone	U_{air}	cm/s	225			
Exposure duration	ED	years	25	Width of source area parallel to wind, or ground water flow direction	W	cm	1500			
				Ambient air mixing zone height	δ_{air}	cm	200			
				Volumetric air content in capillary fringe soils	θ_{acap}	cm^3-air/cm^3-soil	0.038			
				Volumetric air content in vadose zone soils	θ_{av}	cm^3-air/cm^3-soil	0.28			
				Total soil porosity	θ_T	cm^3/cm^3-soil	0.38			
				Volumetric water content in capillary fringe soils	θ_{wcap}	cm^3-H_2O/cm^3-soil	0.342			
				Volumetric water content in vadose zone soils	θ_{wv}	cm^3-H_2O/cm^3-soil	0.12			

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RBSL, outdoor air, commercial land use										
Risk-Based Screening Level	$RBSL_{adj}$	$\mu g/m^3$-*air*	8.42E+00	Diffusion coefficient in air	D_{air}	cm^2/s	0.68	Cross-media volatilization factor	V_{cross}	3.07E-04
Target excess individual lifetime cancer risk	TR	unitless	1.00E-05	Diffusion coefficient in water	D_{wat}	cm^2/s	9.00E-05	Effective diffusion coefficient in soil based on vapor-phase concentration	D_s	5.31E-02
Adult body weight	BW	kg	70	Henry's Law constant	H	cm^3-H_2O/cm^3-*air*	0.37	Effective diffusion coefficient through capillary fringe	D_{cap}	1.35E-04
Averaging time for carcinogens	AT_c	years	70	Thickness of capillary fringe	h_{cap}	cm	5	Effective diffusion coefficient between groundwater and soil surface	D_{ws}	4.30E-03
Inhalation cancer slope factor	SF_i	$(mg/kg\text{-}day)^{-1}$	0.017	Thickness of vadose zone	h_v	cm	168	Risk-Based Screening Level, ambient air, inhalation, commercial exposure	$RBSL_{adj}$	8.42E+00
Inhalation rate	IR_{air}	m^3/day	20	Depth to groundwater	L_{gw}	cm	173	Risk-Based Screening Level, groundwater to ambient air, commercial exposure	$RBSL_{gw-a}$	2.74E+01
Exposure frequency	EF	days/year	250	Wind speed above ground surface in ambient mixing zone	U_{air}	cm/s	225			
Exposure duration	ED	years	25	Width of source area parallel to wind, or ground water flow direction	W	cm	1500			
				Ambient air mixing zone height	δ_{air}	cm	200			
				Volumetric air content in capillary fringe soils	θ_{acap}	cm^3-*air*/cm^3-*soil*	0.038			
				Volumetric air content in vadose zone soils	θ_{av}	cm^3-*air*/cm^3-*soil*	0.26			
				Total soil porosity	θ_T	cm^3/cm^3-*soil*	0.38			
				Volumetric water content in capillary fringe soils	θ_{wcap}	cm^3-H_2O/cm^3-*soil*	0.342			
				Volumetric water content in vadose zone soils	θ_{wv}	cm^3-H_2O/cm^3-*soil*	0.12			

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RBSL, outdoor air, commercial land use										
Risk-Based Screening Level	$RBSL_{am}$	µg/m³-air	4.93E+00	Diffusion coefficient in air	D_{air}	cm^2/s	0.093	Cross-media volatilization factor	V_{vamb}	2.90E-05
Target excess individual lifetime cancer risk	TR	unitless	1.00E-05	Diffusion coefficient in water	D_{wat}	cm^2/s	1.10E-05	Effective diffusion coefficient in soil based on vapor-phase concentration	D_s	7.26E-03
Adult body weight	BW	kg	70	Henry's Law constant	H	cm^3-H_2O/cm^3-air	0.22	Effective diffusion coefficient through capillary fringe	D_{cap}	2.17E-05
Averaging time for carcinogens	AT_c	years	70	Thickness of capillary fringe	h_{cap}	cm	5	Effective diffusion coefficient between groundwater and soil surface	D_{ws}	6.82E-04
Inhalation cancer slope factor	SF_I	$(mg/kg\text{-}day)^{-1}$	0.029	Thickness of vadose zone	h_v	cm	168	Risk-Based Screening Level, ambient air, inhalation, commercial exposure	$RBSL_{soh}$	4.93E+00
Inhalation rate	IR_{air}	m³/day	20	Depth to groundwater	L_{gw}	cm	173	Risk-Based Screening Level, groundwater to ambient air, commercial exposure	$RBSL_{gw\text{-}soh}$	1.70E+02
Exposure frequency	EF	days/year	250	Wind speed above ground surface in ambient mixing zone	U_{air}	cm/s	225			
Exposure duration	ED	years	25	Width of source area parallel to wind, or ground water flow direction	W	cm	1500			
				Ambient air mixing zone height	δ_{air}	cm	200			
				Volumetric air content in capillary fringe soils	θ_{acap}	cm^3-air/cm^3-soil	0.038			
				Volumetric air content in vadose zone soils	θ_{av}	cm^3-air/cm^3-soil	0.26			
				Total soil porosity	θ_T	cm^3/cm^3-soil	0.38			
				Volumetric water content in capillary fringe soils	θ_{wcap}	cm^3-H_2O/cm^3-soil	0.342			
				Volumetric water content in vadose zone soils	θ_{wv}	cm^3-H_2O/cm^3-soil	0.12			

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RBSL, outdoor air, commercial land use										
Risk-Based Screening Level	$RBSL_{oa}$	$\mu g/m^3$-*air*	1.57E+00	Diffusion coefficient in air	D_{air}	cm^2/s	0.74	Cross-media volatilization factor	V_{csoil}	1.19E-04
Target excess individual lifetime cancer risk	TR	unitless	1.00E-05	Diffusion coefficient in water	D_{wat}	cm^2/s	9.70E-05	Effective diffusion coefficient in soil based on vapor-phase concentration	D_s	5.78E-02
Adult body weight	BW	kg	70	Henry's Law constant	H	cm^3-H_2O/cm^3-*air*	0.045	Effective diffusion coefficient through capillary fringe	D_{cap}	5.15E-04
Averaging time for carcinogens	AT_c	years	70	Thickness of capillary fringe	h_{cap}	cm	5	Effective diffusion coefficient between groundwater and soil surface	D_{eff}	1.37E-02
Inhalation cancer slope factor	SF_i	$(mg/kg\text{-}day)^{-1}$	0.091	Thickness of vadose zone	h_v	cm	168	Risk-Based Screening Level, ambient air, inhalation, commercial exposure	$RBSL_{oa-ih}$	1.57E+00
Inhalation rate	IR_{air}	m^3/day	20	Depth to groundwater	L_{gw}	cm	173	Risk-Based Screening Level, groundwater to ambient air, commercial exposure	$RBSL_{gw-oa}$	1.32E+01
Exposure frequency	EF	days/year	250	Wind speed above ground surface in ambient mixing zone	U_{air}	cm/s	225			
Exposure duration	ED	years	25	Width of source area parallel to wind, or ground water flow direction	W	cm	1500			
				Ambient air mixing zone height	δ_{air}	cm	200			
				Volumetric air content in capillary fringe soils	θ_{acap}	cm^3-*air*/cm^3-*soil*	0.038			
				Volumetric air content in vadose zone soils	θ_{av}	cm^3-*air*/cm^3-*soil*	0.26			
				Total soil porosity	θ_T	cm^3/cm^3-*soil*	0.38			
				Volumetric water content in capillary fringe soils	θ_{wcap}	cm^3-H_2O/cm^3-*soil*	0.342			
				Volumetric water content in vadose zone soils	θ_{wv}	cm^3-H_2O/cm^3-*soil*	0.12			

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RBSL, outdoor air, commercial land use										
Risk-Based Screening Level	$RBSL_{oa}$	µg/m³-air	1.19E-01	Diffusion coefficient in air	D_{air}	cm^2/s	0.77	Cross-media volatilization factor	$V_{cm/a}$	9.57E-04
Target excess individual lifetime cancer risk	TR	unitless	1.00E-05	Diffusion coefficient in water	D_{wat}	cm^2/s	1.00E-04	Effective diffusion coefficient in soil based on vapor-phase concentration	D_s	6.01E-02
Adult body weight	BW	kg	70	Henry's Law constant	H	cm^3-H_2O/cm^3-air	1.34	Effective diffusion coefficient through capillary fringe	D_{cap}	1.14E-04
Averaging time for carcinogens	AT_c	years	70	Thickness of capillary fringe	h_{cap}	cm	5	Effective diffusion coefficient between groundwater and soil surface	D_{eff}	3.70E-03
Inhalation cancer slope factor	SF_I	$(mg/kg\text{-}day)^{-1}$	1.2	Thickness of vadose zone	h_v	cm	168	Risk-Based Screening Level, ambient air, inhalation, commercial exposure	$RBSL_{oah}$	1.19E-01
Inhalation rate	IR_{air}	m³/day	20	Depth to groundwater	L_{gw}	cm	173	Risk-Based Screening Level, groundwater to ambient air, commercial exposure	$RBSL_{gw-oah}$	1.25E-01
Exposure frequency	EF	days/year	250	Wind speed above ground surface in ambient mixing zone	U_{air}	cm/s	225			
Exposure duration	ED	years	25	Width of source area parallel to wind, or ground water flow direction	W	cm	1500			
				Ambient air mixing zone height	δ_{air}	cm	200			
				Volumetric air content in capillary fringe soils	θ_{acap}	cm^3-air/cm^3-soil	0.038			
				Volumetric air content in vadose zone soils	θ_{av}	cm^3-air/cm^3-soil	0.26			
				Total soil porosity	θ_T	cm^3/cm^3-soil	0.38			
				Volumetric water content in capillary fringe soils	θ_{wcap}	cm^3-H_2O/cm^3-soil	0.342			
				Volumetric water content in vadose zone soils	θ_{wv}	cm^3-H_2O/cm^3-soil	0.12			

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RBSL, outdoor air, commercial land use										
Risk-Based Screening Level	$RBSL_{bth}$	$\mu g/m^3$-air	1.77E+00	Diffusion coefficient in air	D_{air}	cm^2/s	0.77	Cross-media volatilization factor	V_{vamb}	2.06E-04
Target excess individual lifetime cancer risk	TR	unitless	1.00E-05	Diffusion coefficient in water	D_{wat}	cm^2/s	1.10E-04	Effective diffusion coefficient in soil based on vapor-phase concentration	D_s	6.01E-02
Adult body weight	BW	kg	70	Henry's Law constant	H	cm^3-H_2O/cm^3-air	0.14	Effective diffusion coefficient through capillary fringe	D_{cap}	2.52E-04
Averaging time for carcinogens	AT_c	years	70	Thickness of capillary fringe	h_{cap}	cm	6	Effective diffusion coefficient between groundwater and soil surface	D_{ws}	7.64E-03
Inhalation cancer slope factor	SF_i	$(mg/kg\text{-}day)^{-1}$	0.081	Thickness of vadose zone	h_v	cm	168	Risk-Based Screening Level, ambient air, inhalation, commercial exposure	$RBSL_{bth}$	1.77E+00
Inhalation rate	IR_{air}	m^3/day	20	Depth to groundwater	L_{gw}	cm	173	Risk-Based Screening Level, groundwater to ambient air, commercial exposure	$RBSL_{gw\text{-}bth}$	8.56E+00
Exposure frequency	EF	days/year	250	Wind speed above ground surface in ambient mixing zone	U_{air}	cm/s	225			
Exposure duration	ED	years	25	Width of source area parallel to wind, or ground water flow direction	W	cm	1500			
				Ambient air mixing zone height	δ_{air}	cm	200			
				Volumetric air content in capillary fringe soils	θ_{acap}	cm^3-air/cm^3-soil	0.038			
				Volumetric air content in vadose zone soils	θ_{av}	cm^3-air/cm^3-soil	0.26			
				Total soil porosity	θ_T	cm^3/cm^3-soil	0.38			
				Volumetric water content in capillary fringe soils	θ_{wcap}	cm^3-H_2O/cm^3-soil	0.342			
				Volumetric water content in vadose zone soils	θ_{wv}	cm^3-H_2O/cm^3-soil	0.12			

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