

This spreadsheet calculates total soil concentrations (µg/kg) based on soil vapor concentrations in ppbv
 The shaded values are used as input concentrations for VLEACH

Bulk Density (kg/L)	1.3
Porosity (-)	0.40
Volumetric Water Content (-)	0.15
Fraction of Organic Carbon (-)	0.001

	1,1-DCE	1,1,1-TCA	TCTFA	1,1-DCA	PCE	TCE	1,2-DCP
Molecular Weight (g/mole)	97	133	187.38	99	166	131	113
K _{oc} (L/kg)	65	152	160	30	364	126	27
K _H (atm*m ³ /mole)			0.52	0.0057			
K _H at 20°C (-)	0.870	0.560	21.62	0.237	0.545	0.300	0.096

	Concentration	
	Soil Vapor µg/L	Total Soil µg/kg
1,1-DCE		0.00
1,1,1-TCA		0.0
TCTFA		0.00
1,1-DCA		0.00
PCE		0.00

Equations:

Henry's Law Constant (K_H) Unit Conversion

$$K_{Hdimensionless} = ((K_H)(10^3))/(RT)$$

Where:

- K_{Hdimensionless} = Henry's Law Constant (-)
- K_H = Henry's Law Constant (atm*m³/mole)
- R = Universal Gas Constant (0.08206 L*atm/mole*°K)
- T = Temperature in Degrees Kelvin (293.15 °K)

Soil Vapor Concentration Unit Conversion

$$C_{Vµg/L} = ((ppbv)(MW)(10^{-3}))/RT$$

Where:

- C_{Vµg/L} = total soil vapor concentration (µg/L)
- ppbv = total soil vapor concentration (ppbv)
- MW = molecular weight (g/mole)
- R = Universal Gas Constant (0.08206 L*atm/mole*°K)
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Calculation of Total Soil Concentration from Total Soil-Vapor Concentration

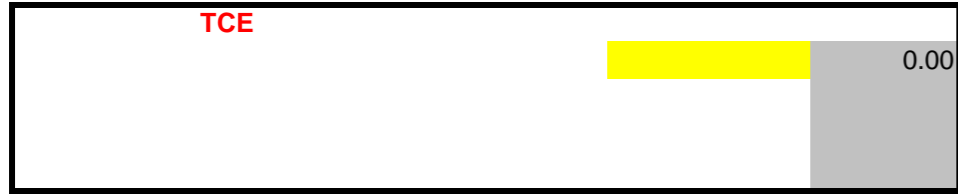
$$C_T = (((K_D)(P_b)/K_H) + (\theta_w/K_H) + (\theta_T - \theta_w))(C_V)/P_b$$

Where:

- C_T = total soil concentration (µg/kg)
- C_V = total soil vapor concentration (µg/L)

INPUT

OUTPUT



K_D = soil-water partitioning distribution coefficient= $(K_{oc})(f_{oc})$ [L/kg]

P_b = bulk density (kg/L)

K_H = Henry's Law Constant (-)

θ_w = volumetric water content (-)

θ_T = total porosity (-)

K_{oc} = organic carbon partition coefficient (L/kg)

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Bulk Density (kg/L)	1.5
Porosity (-)	0.30
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Soil Vapor Concentration Unit Conversion

$$C_{V\mu\text{g}/\text{L}} = ((\text{ppbv})(\text{MW})(10^{-3}))/(\text{RT})$$

Where:

- $C_{V\mu\text{g}/\text{L}}$ = total soil vapor concentration ($\mu\text{g}/\text{L}$)
- ppbv = total soil vapor concentration (ppbv)
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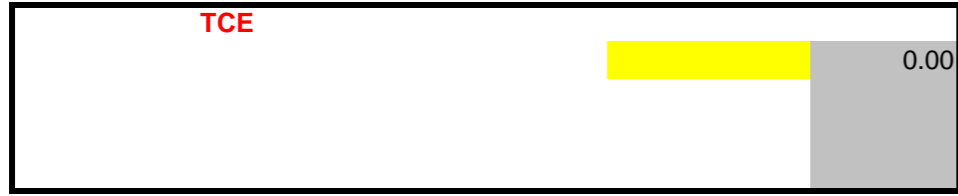
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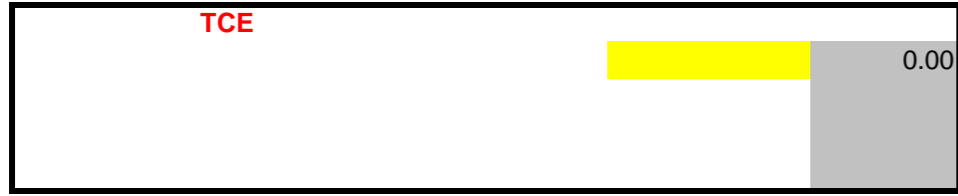
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INPUT
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Bulk Density (kg/L)	1.3
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Fraction of Organic Carbon (-)	0.001

	1,1,2,2-PCA	cis-1,2-DCE	Benzene	Chloroform	PCE	TCE	Vinyl Chloride
Molecular Weight (g/mole)	167.86	96.94	78.11	119.39	165.85	131.4	62.5
K_{oc} (L/kg)	79	29	57	56	300	94	11
K_H (atm*m³/mole)	3.72E-04	0.005	0.005	0.004	0.017	0.011	0.084
K_H at 20°C (-)	0.015	0.208	0.208	0.166	0.707	0.457	3.492

	Concentration		Total Soil $\mu\text{g}/\text{kg}$
	Soil Vapor ppbv	$\mu\text{g}/\text{L}$	
1,1,2,2-PCA			
0-10 ft bgs	40.3	0.28	4.12
10-15 ft bgs	4.9	0.03	0.50
15-35 ft bgs	3.3	0.02	0.34
35-41 ft bgs	137	0.96	14.0

cis-1,2-DCE			
0-10 ft bgs	5590	22.53	20.9
10-15 ft bgs	486	1.96	1.82
15-35 ft bgs	323	1.30	1.21
35-41 ft bgs	14800	59.64	55.3

Benzene			
0-10 ft bgs	40.3	0.13	0.14
10-15 ft bgs	8.6	0.03	0.03
15-35 ft bgs	3.3	0.01	0.01
35-41 ft bgs	137	0.44	0.47

Chloroform			
0-10 ft bgs	40.3	0.20	0.26
10-15 ft bgs	8.3	0.04	0.05
15-35 ft bgs	3.3	0.02	0.02
35-41 ft bgs	137	0.68	0.88

PCE			
0-10 ft bgs	40.3	0.28	0.20
10-15 ft bgs	26.3	0.18	0.13
15-35 ft bgs	26.3	0.18	0.13
35-41 ft bgs	137	0.94	0.68

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Where:

C_T = total soil concentration ($\mu\text{g}/\text{kg}$)

C_v = total soil vapor concentration ($\mu\text{g}/\text{L}$)

TCE			
0-10 ft bgs	687	3.75	2.29
10-15 ft bgs	340	1.86	1.13
15-35 ft bgs	361	1.97	1.20
35-41 ft bgs	7300	39.87	24.3

Vinyl Chloride			
0-10 ft bgs	40.3	0.10	0.01
10-15 ft bgs	6.1	0.02	0.002
15-35 ft bgs	11.6	0.03	0.004
35-41 ft bgs	315	0.82	0.11

K_D = soil-water partitioning distribution coefficient= $(K_{oc})(f_{oc})$ [L/kg]

P_b = bulk density (kg/L)

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