How to relate soil matrix to soil gas samples

Matrix samples are per kilogram, soil gas are per liter...

By Yue Rong, Ph.D.

An environmental site assessment commonly requires soil matrix and soil gas samples for analysis of volatile organic compounds (VOCs). Commonly, concentrations in soil matrix samples are reported in micrograms per kilogram (µg/kg) and for soil gas samples, in micrograms per liter (µg/L). What is the relationship between the two concentration units?

In the theory of VOC partition and equilibrium in the vadose zone, soil concentration can be related to soil gas concentration by the following equation:

$C_T = C_g \bullet [\theta + (n - \theta) \bullet K_H + \rho_b \bullet f_{oc} \bullet K_{oc}] / (\rho_b \bullet K_H)$ (equation one)

Where C_T is the soil concentration in µg/kg, C_g is the soil gas concentration in µg/L, θ is soil water content by volume (dimensionless), n is soil porosity (dimensionless), ρ_b is soil bulk density (g/cm³), f_{oc} is soil organic carbon content (dimensionless), K_H is Henry's Law constant (dimensionless), and K_{oc} is organic carbon partition coefficient (cm³/g).

Now, let CO be the coefficient between C_T and C_g in equation one, hence, $CO = [\theta+(n-\theta)\bullet K_H + \rho_b \bullet f_{oc} \bullet K_{oc}] / (\rho_b \bullet K_H)$. Therefore, equation one becomes:

C_T (µg/kg) = CO X C_g (µg/L) (equation two).

Based on soil physical properties of 55 soil samples obtained in Los Angeles, as summarized in figure one, page 22, we can calculate CO for the average scenario and silt vs. sand scenario.

a) Average CO

Using equation one, and given the median values in figure one (mean is equal to median in the normal distribution) as follows:

ρ_b = 1.746 (g/cm³), θ = 0.167 (—), f_{oc} = 0.00138 (—), n = 0.364 (—), the average COs for common VOCs are calculated in figure two, page 22. On one extreme end, highly volatile compounds with a large value of Henry's Law constant, tend to have low CO values. For instance, vinyl chloride CO = 0.12, which means, by equation two, that if soil gas concentration (C_g) is detected in 100 µg/L, the soil concentration (C_T) would be 12 µg/kg. On the other extreme end, for compounds of low

Yue Rong, Ph.D., is an environmental specialist for the California Regional Water Quality Control Board, Los Angeles Region

Continues on page 22→

How to relate, from page 20

Figure one, right
Figure two, below

Statistics of Soil Parameters from 55 Samples				
	ρ_b (g/cm³)	θ (--)	f_{oc} (--)	n (--)
Distribution	Normal	Normal	Log-Normal	Normal
Minimum	1.2	0.031	0.0002	0.143
Maximum	2.27	0.4	0.015	0.54
Mean	1.746	0.167	0.00247	0.364
Std. Deviation	0.242	0.103	0.00324	0.093
Median	--	--	0.00138	--

Conversion Coefficient between Soil Concentration in µg/kg and µg/L for common VOCs

Compound	K_{oc} (ml/g)	KH (--)	CO (avg)	CO (silt)	CO (sand)
MTBE	38	0.023	6.6	6.3	4.2
Acetone	2	0.0009	109.5	96	52
Methyl Ethyl Ketone (MEK)	5	0.0011	93	82	46
Chloroethane	3	0.387	0.37	0.6	0.14
Benzene	65	0.229	0.92	1.13	0.6
Chloroform	31	0.158	0.99	1.17	0.57
Cis-1,2-dichloroethylene (c-1,2-DCE)	59	0.274	0.76	0.97	0.48
Dichlorodifluoromethane (Freon 12)	58	4.158	0.16	0.41	0.05
1,1-Dichloroethane (1,1-DCA)	30	0.179	0.88	1.1	0.5
1,2-Dichloroethane (1,2-DCA)	14	0.05	2.41	2.43	1.29
Dichloromethane (Methylene Chloride)	9	0.11	1.1	1.24	0.53
1,1,1,2-Tetrachloroethane	54	0.016	10.8	10.2	7.4
Trans-1,2-dichloriethylene (t-1,2-DCE)	59	0.274	0.76	0.97	0.48
1,1,2-Trichloroethane (1,1,2-TCA)	56	0.05	3.6	3.6	2.4
Carbon Tetrachloride	110	0.998	0.36	0.61	0.22
Chlorobenzene	160	0.146	2.28	2.46	1.84
1,1-Dichloroethylene (1,1-DCE)	65	6.237	0.14	0.4	0.04
Ethylbenzene	220	0.328	1.33	1.55	1.08
1,1,2,2-Tetrachloroethane	220	0.021	19.2	18.8	16.6
Tetrachloroethylene (PCE)	660	0.956	1.17	1.41	1.02
Toluene	260	0.274	1.77	1.99	1.49
1,1,1-Trichloroethane (1,1,1-TCA)	150	0.116	2.73	2.88	2.19
Trichloroethylene (TCE)	130	0.371	0.86	1.08	0.62
Trichlorofluoromethane (Freon 11)	160	4.03	0.19	0.45	0.08
1,1,2-Trichloro-trifluoroethane (Freon 113)	160	2.41	0.24	0.5	0.13
Vinyl chloride (VC)	57	29.1	0.12	0.38	0.02
o,m,p - Xylene	240	0.22	2.06	2.26	1.73
1,2-Dichlorobenzene	1100	0.079	20.6	20.7	19.8
1,3-Dichlorobenzene	1200	0.079	22.3	22.4	21.6
1,4-Dichlorobenzene	1200	0.066	26.7	26.7	25.8

volatility (smaller value of Henry's Law constant) CO values are opposite of those of highly volatile compounds. For example, for acetone CO = 109.5, which implies that if soil gas concentration is detected in 100 μg/L, the soil concentration would be 10,950μg/kg. In general, given soil type, for highly volatile compounds, soil gas concentration measured in μg/L is higher than soil concentration measured in μg/kg in terms of values. For less volatile compounds, soil concentration in μg/kg is higher than soil gas concentration in μg/L in terms of values.

However, for those compounds at neither extreme end, soil properties and the individual organic carbon partition coefficient K_{oc} may be the influential factors to CO value. For example, the most common VOC soil contaminants tetrachloroethylene (PCE) and trichloroethylene (TCE) have CO equal to 1.17 and 0.86 respectively, as in figure two. These coefficients imply that soil concentration and soil gas concentration are almost a 1:1 ratio in the type of soils represented by the 55 samples.

b) CO for silty and sandy scenario

Using equation one, and given data from the 55 samples, these soil physical property parameter values are used to calculate CO for silt:

$\rho_b = 1.2$ (g/cm³), $\theta = 0.1$ (—), $f_{oc} = 0.00138$ (—), n = 0.547 (—)

and, for sand:

$\rho_b = 2.27$ (g/cm³), $\theta = 0.1$ (—), $f_{oc} = 0.00138$ (—), n = 0.143 (—)

Results of COs under silt and sand scenarios for common VOCs are also presented in figure two. Comparison of the CO values between silt and sand indicates that CO for sand is always smaller than that for silt among the 29 compounds. Therefore, given a certain amount of soil concentration, soil gas concentration would always be higher in sand than in silt.

In summary, CO value is relatively small for highly volatile compounds in coarse material soil. CO value tends to be larger for less volatile compounds in fine-grained soils. Therefore, in a subsurface investigation, when volatile contaminants are in coarse soil such as sand or gravel, soil gas samples should be analyzed. When less volatile contaminants are in fine-grained material such as silt or clay, soil matrix samples could be better. Other situations, such as volatile contaminant in fine-grained soil or contaminant of low volatility in coarse soil may need calculation of particular CO values to assist in making a decision which soil gas or soil matrix samples should be taken. Calculation of CO values can be very site-specific.■