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:

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

Where $C_T$ is the soil concentration in µg/kg, $C_g$ is the soil gas concentration in µg/L, $\theta$ is soil water content by volume (dimensionless), $n$ is soil porosity (dimensionless), $p_b$ is soil bulk density (g/cm$^3$), $f_{oc}$ is soil organic carbon content (dimensionless), $K_H$ is Henry’s Law constant (dimensionless), and $K_{oc}$ is organic carbon partition coefficient (cm$^3$/g).

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

$C_T (µg/kg) = CO \times C_g (µg/L)$  (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:

$p_b = 1.746$ (g/cm$^3$), $\theta = 0.167$ (—), $f_{oc} = 0.00138$ (—), $n = 0.364$ (—), 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...
### How to relate,
from page 20

**Figure one, right**

**Figure two, below**

<table>
<thead>
<tr>
<th>Statistics of Soil Parameters from 55 Samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_s$ (g/cm$^3$)</td>
</tr>
<tr>
<td>Distribution</td>
</tr>
<tr>
<td>Minimum</td>
</tr>
<tr>
<td>Maximum</td>
</tr>
<tr>
<td>Mean</td>
</tr>
<tr>
<td>Std. Deviation</td>
</tr>
<tr>
<td>Median</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Compound</th>
<th>$K_{oc}$ (mL/g)</th>
<th>KH (--)</th>
<th>CO (avg)</th>
<th>CO (silt)</th>
<th>CO (sand)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M+T+S+C$</td>
<td>3.8</td>
<td>0.0009</td>
<td>109.5</td>
<td>96</td>
<td>52</td>
</tr>
<tr>
<td>Acetone</td>
<td>6</td>
<td>0.0111</td>
<td>93</td>
<td>82</td>
<td>46</td>
</tr>
<tr>
<td>Methyl Ethyl Ketone (MEK)</td>
<td>5</td>
<td>0.347</td>
<td>0.37</td>
<td>0.6</td>
<td>0.14</td>
</tr>
<tr>
<td>Benzene</td>
<td>65</td>
<td>0.229</td>
<td>0.92</td>
<td>1.13</td>
<td>0.6</td>
</tr>
<tr>
<td>Chloroform</td>
<td>31</td>
<td>0.158</td>
<td>0.99</td>
<td>1.17</td>
<td>0.57</td>
</tr>
<tr>
<td>cis-1,2-dichloroethylene (c-1,2-DCE)</td>
<td>59</td>
<td>0.274</td>
<td>0.76</td>
<td>0.97</td>
<td>0.48</td>
</tr>
<tr>
<td>Dichlorodifluoromethane (Freon 12)</td>
<td>58</td>
<td>1.158</td>
<td>0.16</td>
<td>0.41</td>
<td>0.05</td>
</tr>
<tr>
<td>1,1-Dichloroethane (1,1-DCA)</td>
<td>30</td>
<td>0.197</td>
<td>0.88</td>
<td>1.1</td>
<td>0.5</td>
</tr>
<tr>
<td>1,2-Dichloroethane (1,2-DCA)</td>
<td>14</td>
<td>0.05</td>
<td>2.41</td>
<td>2.48</td>
<td>1.09</td>
</tr>
<tr>
<td>Dichloromethane (Methylene Chloride)</td>
<td>9</td>
<td>0.11</td>
<td>1.1</td>
<td>1.24</td>
<td>0.53</td>
</tr>
<tr>
<td>1,1,1-Trichloroethane</td>
<td>6</td>
<td>0.016</td>
<td>10.8</td>
<td>10.2</td>
<td>1.3</td>
</tr>
<tr>
<td>Trans-1,2-dichloroethylene (t-1,2-DCE)</td>
<td>59</td>
<td>0.274</td>
<td>0.76</td>
<td>0.97</td>
<td>0.48</td>
</tr>
<tr>
<td>1,1,2-Trichloroethane (1,1,2-TCA)</td>
<td>56</td>
<td>0.05</td>
<td>3.6</td>
<td>3.6</td>
<td>2.4</td>
</tr>
<tr>
<td>Carbon Tetrachloride</td>
<td>110</td>
<td>0.998</td>
<td>0.36</td>
<td>0.61</td>
<td>0.22</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>160</td>
<td>0.146</td>
<td>2.28</td>
<td>2.45</td>
<td>1.84</td>
</tr>
<tr>
<td>1,1-Dichloroethylene (1,1-DCE)</td>
<td>65</td>
<td>6.237</td>
<td>0.14</td>
<td>0.4</td>
<td>0.04</td>
</tr>
<tr>
<td>Phenol</td>
<td>220</td>
<td>0.328</td>
<td>1.33</td>
<td>1.55</td>
<td>1.08</td>
</tr>
<tr>
<td>1,1,2,2-Tetrachloroethane</td>
<td>220</td>
<td>0.021</td>
<td>19.2</td>
<td>18.8</td>
<td>16.6</td>
</tr>
<tr>
<td>Tetrachloroethylene (PCE)</td>
<td>660</td>
<td>0.956</td>
<td>1.17</td>
<td>1.41</td>
<td>1.02</td>
</tr>
<tr>
<td>Toluene</td>
<td>260</td>
<td>0.274</td>
<td>1.77</td>
<td>1.99</td>
<td>1.49</td>
</tr>
<tr>
<td>1,1-Trichloroethane (1,1-TCA)</td>
<td>150</td>
<td>0.116</td>
<td>2.73</td>
<td>2.88</td>
<td>2.19</td>
</tr>
<tr>
<td>Trichloroethylene (TCE)</td>
<td>130</td>
<td>0.371</td>
<td>0.86</td>
<td>1.08</td>
<td>0.62</td>
</tr>
<tr>
<td>Trichlorofluoromethane (Freon 11)</td>
<td>160</td>
<td>4.03</td>
<td>0.19</td>
<td>0.45</td>
<td>0.08</td>
</tr>
<tr>
<td>1,1,2-Trichloro-trifluoroethane (Freon 113)</td>
<td>160</td>
<td>2.41</td>
<td>0.24</td>
<td>0.5</td>
<td>0.13</td>
</tr>
<tr>
<td>Vinyl chloride (VC)</td>
<td>57</td>
<td>28.1</td>
<td>0.12</td>
<td>0.38</td>
<td>0.02</td>
</tr>
<tr>
<td>o,m,p - Xylene</td>
<td>240</td>
<td>0.22</td>
<td>2.06</td>
<td>2.26</td>
<td>1.73</td>
</tr>
<tr>
<td>1,2-Dichlorobenzene</td>
<td>1700</td>
<td>0.079</td>
<td>20.6</td>
<td>20.7</td>
<td>12.8</td>
</tr>
<tr>
<td>1,3-Dichlorobenzene</td>
<td>1200</td>
<td>0.079</td>
<td>22.3</td>
<td>22.4</td>
<td>21.6</td>
</tr>
<tr>
<td>1,4-Dichlorobenzene</td>
<td>1200</td>
<td>0.065</td>
<td>28.7</td>
<td>26.7</td>
<td>25.8</td>
</tr>
</tbody>
</table>

22 June July 1996 Soil & Groundwater Cleanup
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:

$\rho_b = 1.2 \text{ (g/cm}^3\text{)}, \theta = 0.1 (-), f_{OC} = 0.00138 (-), n = 0.547 (-)$

and, for sand:

$\rho_b = 2.27 \text{ (g/cm}^3\text{)}, \theta = 0.1 (-), f_{OC} = 0.00138 (-), n = 0.143 (-)$

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.\[\text{Write In 696}\]