Remediation of soils and groundwater
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Problem set #1: contaminant properties

Problem 1:

closed bottle 10 mL gas = 10^{-5} m^3 = V_G
90 mL water = $9 \cdot 10^{-5}$ m^3 = V_L

T = 20 °C
M_S = 36 mg solid with specific gravity of 1

$$36 \cdot 10^{-3} g \cdot \frac{1cm^3}{1g} \quad \rightarrow \quad V_s = 3.6 \cdot 10^{-8} \text{ m}^3$$

f_{OC} = 0.1
10 mg PCE
MW_{PCE} = 166
K_H' = 0.6
Log K_{OW} = 2.67

Mass balance:

$$m_{PCE,aq} + m_{PCE,g} + m_{PCE,s} = m_{PCE,t} = 10^{-2} g \qquad (1)$$

Partitioning coefficients:

$$K_H' \cdot \frac{V_G}{V_L} \cdot m_{PCE,aq} = m_{PCE,g} \qquad (2)$$

$$\frac{K_D \cdot m_{PCE,aq} \cdot M_S}{V_L} = m_{PCE,s} \qquad (3)$$

Calculating K_D

$$\log K_{OC} = 0.989 \cdot \log K_{OW} - 0.346 = 2.29$$

$$K_D = f_{OC} \cdot K_{OC} = 19.7 \frac{m^3}{g}$$

Three equations and three unknowns:

From equation (1):

$$m_{PCE,aq} + \frac{K'_H \cdot V_G}{V_L} \cdot m_{PCE,aq} + \frac{K_D \cdot M_S}{V_L} \cdot m_{PCE,aq} = 10^{-2} g = m_{PCE}$$

$$m_{PCE,aq} = \frac{10^{-2} g}{\frac{0.6 \cdot 10^{-5} m^3}{9 \cdot 10^{-5} m^3} + \frac{19.7 \frac{m^3}{g} \cdot 36 \cdot 10^{-3} g}{9 \cdot 10^{-5} m^3} + 1} = \frac{10^{-2} g}{0.0666 + 7880 + 1}$$

$$m_{PCE,aq} = 1.27 \cdot 10^{-6} g$$
$$m_{PCE,s} = 7880 \cdot 1.27 \cdot 10^{-6} g = 1.00 \cdot 10^{-2} g$$
$$m_{PCE,g} = 0.0666 \cdot 5.6 \cdot 10^{-3} g = 8.46 \cdot 10^{-8} g$$

Problem 2:

$m_{cont,total} = m_{cont,g} + m_{cont,aq}$
$m_{cont,total} = C_{cont,total} V_L = C_{cont,aq} K_H' V_G + C_{cont,aq} V_L$

$$C_{cont,\ aq} = \frac{C_{cont,\ total} \cdot V_L}{K_H' \cdot V_G + V_L}$$

$C_{benz,aq} = 34.2$ µg/L

$C_{tol,aq} = 32.1$ µg/L

$C_{ethylbenz,aq} = 25.6$ µg/L

$C_{xyl,aq} = 26.2$ µg/L

The actual concentration in the aqueous phase is much lower than the intended concentration. This solution needs to be stored with minimal headspace to minimize the volatilization of the compounds.

Problem 3:

$C_{benz,s,initial} = 900$ mg/kg dry soil
$K_D = 0.02\ m^3/kg$
Solids concentration = 40 kg dry soil/m^3 slurry
V_T = volume of slurry = 500 m^3
$\rho_s = 2{,}000\ kg/m^3$
assume no headspace

a- What is V_L?
$M_S = \frac{40 kg}{m^3 slurry} \cdot 500\ m^3$ slurry= 20,000 kg soil
$V_S = 20{,}000\ kg \cdot \frac{1 m^3}{2{,}000 kg} = 10\ m^3$
$V_L = 490\ m^3$

b - what is $C_{benz,aq}$?
$m_{benz,total} = m_{benz,s} + m_{benz,aq}$
$m_{benz,total} = C_{benz,s,initial} \cdot M_s = C_{benz,s} \cdot M_S + C_{benz,aq} \cdot V_L = C_{benz,aq} K_D M_S + C_{benz,aq} V_L$

$$C_{benz,aq} = \frac{C_{benz,initial} \cdot M_s}{K_D \cdot M_s + V_L} = \frac{900 \frac{mg}{kg} \cdot 20{,}000 kg \cdot \frac{1g}{10^3\ mg}}{0.02 \frac{m^3}{kg} \cdot 20{,}000\ kg + 490 m^3} = 20.2 \frac{g}{m^3}$$

Problem 4:

A – In a river
C_{SS} = 10 mg/L
$K_{OW} = 10^6$ (PCB)
$\rho_S = 1\ g/cm^3$
f_{OC} = 0.1

What is the distribution of PCB between water and suspended solids?

$$K_D = \frac{C_{i,s}}{C_{i,aq}} \frac{[g/g]}{[g/m^3]} = 0.63 \cdot 10^{-6} \cdot f_{OC} \cdot K_{OW} = 6.3 \cdot 10^{-2} \frac{m^3}{g}$$

Fraction in the solid phase:

$$f_{PCB,s} = \frac{m_{PCB,s}}{m_{PCB,s} + m_{PCB,aq}} = \frac{\frac{m_{PCB,s}}{m_{PCB,aq}}}{\frac{m_{PCB,s}}{m_{PCB,aq}} + 1}$$

$$\frac{m_{PCB,s}}{m_{PCB,aq}} = K_D \cdot C_{SS} = 6.3 \cdot 10^{-2} \frac{m^3}{g} \cdot \frac{10mg}{L} \cdot \frac{1'000L}{1m^3} \cdot \frac{1g}{1'000mg}$$
$$= 0.63 \frac{g\ PCB\ on\ solid}{g\ PCB\ in\ solution}$$

$$f_{PCB,s} = \frac{0.63}{1.63} = 0.39$$

Comment: over 1/3 of the PCB is on solids even if the solids represent 0.001 % of the total volume

B - For carbon tetrachloride CCl_4 (CT)
K_{OW} = 440
$\rho_S = 1.1\ g/cm^3$
f_{OC} = 0.02

$$K_D = 0.63 \cdot 10^{-6} \cdot f_{OC} \cdot K_{OW} = 5.5 \cdot 10^{-6} \frac{m^3}{g}$$

Dimensionless partitioning coefficient:

$$K_p = \frac{C_{CT,s}\ in \frac{g}{m_S^3}}{C_{CT,aq}\ in \frac{g}{m_{aq}^3}}$$

$$K_p = K_D . \rho_s = 5.5 \cdot 10^{-6} \frac{m^3}{g}\ \ 1.1 \frac{g}{cm^3} \frac{10^6\ cm^3}{m^3} = 6.1\ [-]$$

C - Mass distribution

$V_S/V_T = 10^{-4}$; an approximation is that $V_S/V_L \sim 10^{-4}$

$$\frac{m_{CT,s}}{m_{CT,aq}} = K_p \frac{V_S}{V_L} = 6.1\ 10^{-4}$$

For CT, the distribution between solid and aqueous phase is very different as compared to PCBs. This is due to the difference in K_{OW}. PCBs have a high K_{OW} because they are hydrophobic and tend to associate with organic matter.