Lecture Notes 1

Slides 33 and 34 – Problem 1

$$\boldsymbol{K_{OC} = 182\frac{L}{kg}}$$
$$\boldsymbol{f_{OC} = 0.02}$$
$$\boldsymbol{C_{i,aq} = 20\frac{mg_{tol}}{L}}$$
$$\boldsymbol{\varepsilon = 0.35}$$

In an aquifer (= saturated) there is only two phases: solid and liquid.

First, we consider $\boldsymbol{\rho_b = 1.6\frac{g}{cm^3}}$we would like to calculate $\mathbf{C_{i,s}}$

Given that we have $\mathbf{C_{i,aq}}$, we only need K_D

$$K_D = K_{OC} * f_{OC} = 3.64\frac{L}{kg}\ \frac{1\ kg}{1000\ g}\frac{1\ m^3}{1\ 000\ L} = 3.64 * 10^{-6}\frac{m^3}{g}$$
$$K_D = \frac{C_{i,s}}{C_{i,aq}}$$

➔ $C_{i,s} = K_D C_{i,aq} = 3.64 * 10^{-6}\frac{m^3}{g} 20\frac{mg_{tol}}{L}\ \frac{1000\ L}{m3} = 0.0728\frac{mg_{tol}}{g}\frac{1000\ g}{1\ kg} = 72.8\frac{mg_{tol}}{kg\ dry\ soil}$

We consider 1 m^3 of aquifer => V_T

$$M_S = mass\ of\ dry\ solid = V_T\rho_b = 1\ m^3\ 1.6\ \frac{g}{cm^3}\frac{10^6 cm^3}{m^3}\frac{1\ kg}{1000\ g} = 1{,}600\ kg$$

$m_{i,s} = C_{i,s}M_S = 72.8\frac{mg_{tol}}{kg}\ 1{,}600\ kg = 116.48\ g_{tol}$ in 1 m^3 of aquifer

Second, we consider $\boldsymbol{\rho_{wb} = 1.6\frac{g}{cm^3}}$, we need to recalculate the mass of dry solid in a cubic meter of aquifer.

$$M_s + M_L = V_T\rho_{wb}$$

$$M_L = V_L\rho_{water} = 0.35 * 1\ m^3 * 997\frac{kg}{m^3} = 349\ kg$$
$$M_s = 1{,}600 - 349 = 1{,}251\ kg$$

$$m_{i,s} = C_{i,s}M_s = 72.8 * 1{,}251 = 91\ g_{tol}$$

Less toluene is sorbed on the solid phase because there is less solid phase in the cubic meter of aquifer if the wet bulk density is considered.

Let's calculate what the real ρ_{wb} should be if ρ_b = 1.6 g/cm^3 and the porosity is $\boldsymbol{\varepsilon} = 0.35$

$$\rho_{wb} = \frac{M_s + M_L}{V_T} = \frac{M_S}{V_T} + \frac{M_L}{V_T} = \rho_b + \frac{M_L}{V_T} = 1.6\ \frac{g}{cm^3} + \frac{349\ kg}{1\ m^3} * \frac{1000g}{1\ kg} * \frac{1m^3}{10^6 cm^3}$$
$$= 1.6\ \frac{g}{cm^3} + 0.349\ \frac{g}{cm^3} = 1.949\ \frac{g}{cm^3}$$

$$\boxed{\rho_{wb} = 1.949\ \frac{g}{cm^3}}$$

Problem 2 (slide 36)

pH=12 => [OH-] = 10^{-2} M

$$[Ca^{2+}] = \frac{K_{sp}}{[OH^-]^2} = \frac{6.5 * 10^{-6}}{10^{-4}} = 0.065\ M$$

This means that Ca^{2+} at this concentration (equivalent to 0.065 mol/L * 40 g/mol= 2.6 g/L) is at equilibrium with the $Ca(OH)_2$ solid phase at this pH. So, if you have solid $Ca(OH)_2$ in water (at any amount), the concentration of calcium at equilibrium will be 2.6 g/L (0.065 mol/L) at pH 12.

If we want to know how much $Ca(OH)_2$ we will be able to dissolve in water, then, it will be 0.065 moles per L (it should be stoichiometric with dissolved calcium). However, we like to know how much mass of calcium hydroxide can be dissolved and considering the MW of this compound is 74 g/mol, we get:

$$soluble\ calcium\ hydroxide = 0.065\ \frac{mol}{L} * \frac{74\ g}{mol} = 4.81\ {}^{g}/_{L}$$

You can add 4.81 grams of $Ca(OH)_2$ to one liter of water and it will dissolve at pH 12. If you add more, the excess (more than 4.81 g) will not dissolve and remain in solution. (this is assuming that the pH is buffered at pH 12 and not impacted by the dissolution of the compound)