Lecture Notes week 9

Slide 24 – Example 1

Toluene: $C_6H_5CH_3$

Groundwater properties:

C_{aq} = 20 mg/L= 0.02 kg/m^3

f_{oc} = 0.02

ρ_b = 1.6 g/cm^3=1,600 kg/m^3

K_D = 6.76x10^{-6} m^3/g * 1000g/kg= 6.76x10^{-3} m^3/kg

DO = 4 mg/L

ϵ = 0.35

Total mass of toluene present (we consider V_T = 1 m^3 of aquifer):

$$m_{toluene} = C_{aq}V_T(\epsilon + \rho_b K_D) = C_{aq}(\epsilon + \rho_b K_D)$$

$$= 0.02\frac{kg}{m^3}\left(0.35\,m^3 + 1{,}600\frac{kg}{m^3} * 6.76 * \frac{10^{-3}m^3}{kg}\right) = 0.2232\,kg = 223.3\,g$$

$MW_{toluene}$=12*7+8= 92 g/mol

$$n_{toluene} = \frac{m_{toluene}}{M_{toluene}} = \frac{223.3}{12 * 7 + 8} = 2.43\,mol$$

Quantity of oxygen needed:

$C_6H_5CH_3 + 9O_2 \rightarrow 4H_2O + 7CO_2$

$$n_{O_2} = 9 * 2.43 = 21.85\,mol$$

$$m_{O_2} = 699.1\,g$$

Quantity of oxygen available:

$$m'_{O_2} = DO * V_L = 4\frac{mg}{L} * 350\,L * \frac{1g}{1000\,mg} = 1.4\,g$$

A lot of additional oxygen is needed:

$$\frac{m_{O_2}}{m'_{O_2}} \sim 500$$

Slide 37 - Example 2

Groundwater properties:

Diameter : 25 m

Height : 10 m

n_{TCE} = 100 mol

ϵ = 0.3

f_{OC} = 0.2

LogK_{ow} = 2.42

ρ_b = 1.5 g/cm^3

Halorespiration:

b = 0.01 d^{-1}

K_s = 3 mg/L

Y = 0.6 mg biomass/mg substrate

k = 0.4 mg substrate/(mg biomass.d)

1) **Can we use halorespiration?**

TCE concentration in groundwater:

$m_{TCE} = n_{TCE} M_{TCE} = 100 * 131.4 = 13.1\ kg$

$V_T = \frac{25^2}{4} * \pi * 10 = 4{,}908\ m^3$

$V_L = 0.3 * 4{,}908 = 1{,}472\ m^3$

$M_S = 4{,}908 * 1{,}500 = 7{,}362\ t$= 7.36 * 10^9 g

For K_D calculation we are using Karickoff relation: $K_D \left[\frac{m^3}{g}\right] = 0.63 * 10^{-6} * f_{oc} * K_{ow}$

$K_D = 0.63 * 10^{-6} * 10^{2.42} * 0.2 = 3.3 * 10^{-5} \frac{m^3}{g}$

$C_{TCE,aq} = \frac{m_{TCE}}{V_L + K_D M_S} = \frac{13.1\ kg * 1000\ g/kg}{1{,}472\ m^3 + 7.36 * 10^9 g * 3.3 * 10^{-5}\ m^3/g} = 0.05 \frac{g}{m^3} = 0.05 \frac{mg}{L}$

Minimum TCE concentration to support growth:

$C_{min} = \frac{bK_s}{Yk - b} = 0.01 * \frac{3}{0.6 * 0.4 - 0.01} = 0.13 \frac{mg}{L}$

Halorespiration is not possible because the concentration is below the minimum concentration for growth.

2) **If methanotrophic cometabolism, what total amount of dissolved O_2 is needed?**

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

100 moles of TCE → 500 moles of CH_4 → 1,000 moles O_2

$$C_{O_2,aq} = \frac{1{,}000\ mol * 32 \frac{g}{mol}}{1{,}472\ m^3 * 1{,}000 \frac{L}{m^3}} = 21.7\ mg/L$$

$C_{O_2,aq} > C_{O_2,saturation}$ $(\sim 9\ mg/L)$ so additional oxygen needs to be provided