

Lecture Notes week 9

Slide 24 – Example 1

Toluene: $C_6H_5CH_3$

Groundwater properties:

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

$$f_{oc} = 0.02$$

$$\rho_b = 1.6 \text{ g/cm}^3 = 1,600 \text{ kg/m}^3$$

$$K_D = 6.76 \times 10^{-6} \text{ m}^3/\text{g} * 1000 \text{ g/kg} = 6.76 \times 10^{-3} \text{ m}^3/\text{kg}$$

$$DO = 4 \text{ mg/L}$$

$$\epsilon = 0.35$$

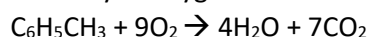
Total mass of toluene present (we consider $V_T = 1 \text{ m}^3$ of aquifer):

$$\begin{aligned} m_{toluene} &= C_{aq} V_T (\epsilon + \rho_b K_D) = C_{aq} (\epsilon + \rho_b K_D) \\ &= 0.02 \frac{\text{kg}}{\text{m}^3} \left(0.35 \text{ m}^3 + 1,600 \frac{\text{kg}}{\text{m}^3} * 6.76 * \frac{10^{-3} \text{ m}^3}{\text{kg}} \right) = 0.2232 \text{ kg} = 223.3 \text{ g} \end{aligned}$$

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

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

Quantity of oxygen needed:



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

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

Quantity of oxygen available:

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

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

$$n_{TCE} = 100 \text{ mol}$$

$$\epsilon = 0.3$$

$$f_{OC} = 0.2$$

$$\text{Log}K_{ow} = 2.42$$

$$\rho_b = 1.5 \text{ g/cm}^3$$

Haloerespiration:

$$b = 0.01 \text{ d}^{-1}$$

$$K_s = 3 \text{ mg/L}$$

$$Y = 0.6 \text{ mg biomass/mg substrate}$$

$$k = 0.4 \text{ mg substrate/(mg biomass.d)}$$

1) Can we use halorespiration?

TCE concentration in groundwater:

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

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

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

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

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

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

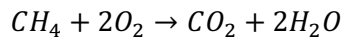
$$C_{TCE,aq} = \frac{m_{TCE}}{V_L + K_D M_S} = \frac{13.1 \text{ kg} * 1000 \frac{\text{g}}{\text{kg}}}{1,472 \text{ m}^3 + 7.36 * 10^9 \text{ g} * 3.3 * 10^{-5} \frac{\text{m}^3}{\text{g}}} = 0.05 \frac{\text{g}}{\text{m}^3} = 0.05 \frac{\text{mg}}{\text{L}}$$

Minimum TCE concentration to support growth:

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

Haloirespiration 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?



100 moles of TCE $\rightarrow$ 500 moles of $CH_4 \rightarrow$ 1,000 moles O_2

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

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