Lecture Notes week 8

Example 1: in situ bioremediation

All units should be consistent. Use: m^3 for volume; kg for mass; seconds for time; m for distance.

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= 0.004 kg/m^3
ϵ = 0.35

The goal of the exercise is to identify how much DO is needed to degrade the toluene and whether the existing dissolved oxygen in the aquifer is sufficient or more is needed.

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

$$m_{toluene} = C_{aq}V_L + C_sM_S$$

$$= C_{aq}V_T\epsilon + C_{aq}K_D\rho_bV_T = C_{aq}V_T(\epsilon + \rho_bK_D) = 0.02\frac{kg}{m^3}\left(0.35\ m^3 + 1{,}600\frac{kg}{m^3} * 6.76 * \frac{10^{-3}m^3}{kg}\right)$$

$$m_{toluene} = 0.2232\ kg$$

Number of moles of toluene present
$MW_{toluene}$=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 (assuming full oxidation to CO_2)

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

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

$$m_{O_2} = 0.699\ kg$$

Quantity of oxygen available:

$$m'_{O_2} = DO * V_L = 0.004\frac{kg}{m^3} * 0.350\ m^3 = 0.0014\ kg$$

A lot of additional oxygen is needed:

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

Example 2

All units should be consistent. Use: m^3 for volume; kg for mass; seconds for time; m for distance.

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= 1500 kg/m^3

Halorespiration:
b = 0.01 d^{-1}=0.01/86400 (s/d)= 1.16*10^{-7} s^{-1}
K_s = 3 mg/L= 0.003 kg/m^3
Y = 0.6 mg biomass/mg substrate= 0.6 kg biomass/kg substrate
k = 0.4 mg substrate/(mg biomass.d)= 0.4 mg substrate/(mg biomass.d)*1d/86400 s= 4.63*10^{-6} kg substrate/(kg biomass. s)

1) Can we use halorespiration?

TCE concentration in groundwater:

$m_{TCE} = n_{TCE} M_{TCE} = 100 * 131.4 = \ 13.14\ kg$

$V_T = \frac{25^2}{4} * \pi * 10 = 4{,}909\ m^3$

$V_L = 0.3 * 4{,}909 = 1{,}473\ m^3$

$M_S = 4{,}909 * 1{,}500 = 7.36 * 10^6$ kg

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

$$K_D = 0.63 * 10^{-6} * 10^{2.42} * 0.2 * \frac{1000g}{1kg} = 3.31 * 10^{-2} \frac{m^3}{kg}$$

$$C_{TCE,aq} = \frac{m_{TCE}}{V_L + K_D M_S} = \frac{13.14\ kg}{1{,}473\ m^3 + 7.36 * 10^6 kg * 3.31 * 10^{-2}\ {}^{m^3}/_{kg}} = 5.38 * 10^{-5} \frac{kg}{m^3}$$

Minimum TCE concentration to support growth:

$$C_{min} = \frac{bK_s}{Yk - b} =$$

$$C_{min} = \frac{1.16 * 10^{-7} s^{-1} * 0.003 \frac{\text{kg}}{\text{m}^3}}{0.6 \frac{kg\ biomass}{kg\ TCE} * 4.63 * \ 10^{-6} \frac{kg\ TCE}{kg\ biomass.\ s} - 1.16 * 10^{-7}\ s^{-1}} = 1.31 * 10^{-4} \frac{kg}{m^3}$$

Halorespiration is not possible because the concentration in solution is below the minimum concentration for growth. Therefore, microbes will not be able to grow on this substrate and remediate the site.

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

Cometabolism entails growth of CH_4 and O_2 and fortuitous reaction with toluene.

We know that we will need 5 moles of methane for every mole of toluene degraded.
However, how much O_2 will be needed?
We start by calculating the stoichiometry of methane to O_2

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

100 moles of TCE → 500 moles of CH_4 → 1,000 moles O_2
The total amount of dissolved O_2 needed

$m_{O_2,aq} = 1{,}000\ mol * 32 \frac{g}{mol} * \frac{1\ kg}{1000\ g} = 32$ kg

In the volume of water available, (V_L=1473 m^3), this would mean a concentration of

$$C_{O_2,aq} = \frac{32kg}{1473m^3} = 0.022\ kg/m^3$$

$C_{O_2,aq} > C_{O_2,saturation}$ ($\sim 9\,mg/L = 0.009\ kg/m^3$) so additional oxygen needs to be provided