Lecture Notes week 9

Example 1: In-situ chemical oxidation

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

How much potassium permanganate is needed to oxidize all the tetrachloroethylene in the aquifer with the following characteristics?
Areal extent of the plume: 20 m^2
Thickness of the plume: 2 m
V_T=40 m^3
Average PCE concentration: $C_{PCE,aq}$ = 400 mg/L= 0.4 kg/m^3
Aquifer porosity: ϵ = 0.35
Organic content fraction: f_{oc} = 0.02
Dry bulk density: ρ_b = 1.6 g/cm^3= 1600 kg/m^3

$$K_{oc} = 1.55 * 10^2 \frac{L}{kg} \rightarrow K_D = f_{oc} * K_{oc} = 3.1 \frac{L}{kg} = 3.1 \frac{L}{kg} \frac{1\,m^3}{1{,}000\,L} = 3.1 * 10^{-3} \frac{m^3}{kg}$$

1) How much PCE in the plume?

$$V_L = V_T \epsilon = 20\ m^2 * 2\ m * 0.35 = 14\ \mathrm{m}^3$$

$$M_S = \rho_b * V_T = 1{,}600 \frac{kg}{m^3} * 20\ m^2 * 2\ m = 64{,}000\ \mathrm{kg}$$

$$m_{PCE,tot} = C_{PCE,aq} V_L + C_{PCE,s} M_S = C_{PCE,aq}(V_L + K_D M_S)$$

$$= 0.4 \frac{kg}{m^3} \left(14\ m^3 + 3.1 * 10^{-3} \frac{m^3}{kg} * 64{,}000\ kg \right) = 85.0\ \mathrm{kg}$$

2) Oxidation reaction

Half-reactions:

$$C_2Cl_4 + 4H_2O \rightarrow 2CO_2 + 4Cl^- + 8H^+ + 4e^-$$

$$MnO_4^- + 3e^- + 4H^+ \rightarrow MnO_2 + 2H_2O$$

Complete reaction :

$$3C_2Cl_4 + 4H_2O + 4MnO_4^- \rightarrow 6CO_2 + 12Cl^- + 8H^+ + 4MnO_2$$

We need 4 moles of potassium permanganate for 3 moles of tetrachloroethylene.

In the soil, there is:

$$n_{PCE} = \frac{85\ kg}{166 \frac{\mathrm{g}}{\mathrm{mol}}} * \frac{1000 g}{1\ kg} = 512.0\ \mathrm{mol}$$

So we need:

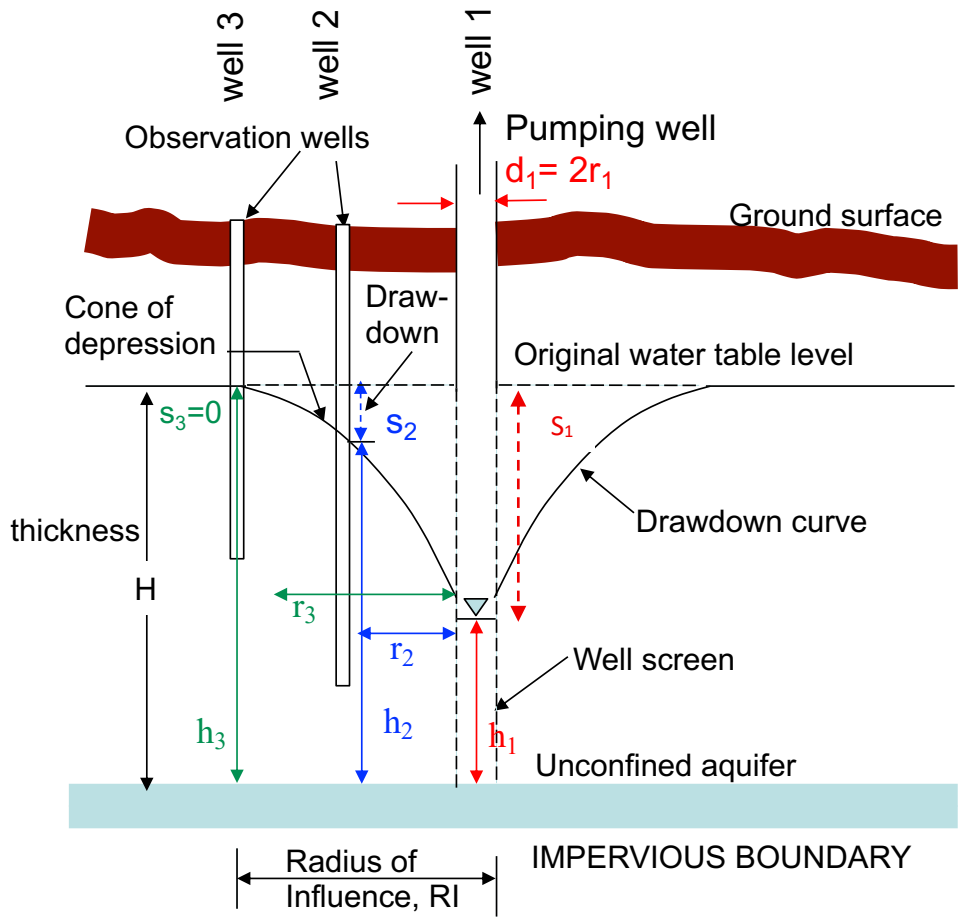
$$n_{KMnO_4} = n_{PCE} * \frac{4}{3} = 682.6\ \mathrm{mol}$$

$$m_{KMnO_4} = 682.6\ \mathrm{mol} * 158 \frac{\mathrm{g}}{\mathrm{mol}} * \frac{1kg}{1000g} = 107.8\ \mathrm{kg}\ KMnO_4$$

This is the minimum amount of oxidant needed. Depending on the organic matter content, the amount will need to be multiplied by 2-10 to be effective.

Example 2: Pump and Treat

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



$$Q = \frac{\pi * K\,(h_2^2 - h_1^2)}{\ln(r_2/r_1)}$$

Aquifer thickness: H=12.2 m
Well diameter: d_1 = 0.1 → r_1 = 0.05 m
Q = 0.15 m^3/min= 0.15 m^3/min *1 min/60s= 0.0025 m^3/s
K = 8.2 m/day= 8.2m/day * 1d/86400 s= $9.5*10^{-5}$ m/s
r_2 = 3 m
s_2= 1.5 m
h_2 = aquifer thickness- drawdown= 12.2 – 1.5 = 10.7 m

1) The drawdown at the well 3m away is 1.5m. What is the drawdown at the pumping well (s_1)?

$$h_1 = \sqrt{h_2^2 - \frac{Q * \ln\left(\frac{r_2}{r_1}\right)}{\pi K}} = \sqrt{10.7^2 - \frac{0.0025\frac{m^3}{s}\ln\left(\frac{3}{0.05}\right)}{9.5 * 10^{-5}\frac{m}{s} * \pi}} = 8.95\ m$$

$$s_1 = 12.2 - 8.95 = 3.25\ m$$

2) What is the radius of influence of the pumping well (r_3=RI)?

We are looking for h_3 = 12.2 m (i.e, no impact on the water level at the radius of influence, s_3=0):

$$\ln\left(\frac{r_3}{r_1}\right) = \frac{\pi * K * (h_3^2 - h_1^2)}{Q} = \frac{\pi * 9.5 * 10^{-5}\frac{m}{s} * (12.2^2 - 8.95^2)m^2}{0.0025\frac{m^3}{s}} = 8.2$$

$$r_3/r_2 = e^{8.2} = 3640.9$$

$$r_3 = 3640.9 * 0.05m = 182.0\ m$$

Example 3: Permeable Reactive Barrier

All units should be consistent. Use: L for volume; hours for time; m for distance

Cr(VI) reduction in PRB.
ε_{PRB}= 0.3 [-]
Hydraulic conductivity of the aquifer K=2m/d=2 m/d* 1d/24h= 8.3* 10^{-2} m.h^{-1}
Hydraulic gradient across the PRB i=1.2 [-]
PRB porosity ε= 0.3 [-]
Rate of reduction k= 0.5 h^{-1}= 0.5 h^{-1}
$C_{aq,initial}$= 2 µM
$C_{aq,final}$= 0.2 µM

What is the residence time needed?

$$t_{res} = \frac{-\ln(\frac{C_{final}}{C_{initial}})}{k} = \frac{-\ln\left(\frac{2*10^{-6}}{2*10^{-7}}\right)}{0.5\ h^{-1}} = 4.6\ h$$

What is the water velocity in the PRB?

$$v = \frac{K*i}{\epsilon_{PRB}} = \frac{8.3*10^{-2}\ m.h^{-1}*1.2}{0.3} = 0.332\ m.h^{-1}$$

What is the thickness of the PRB needed?
Using a safety factor of 3.5

⇨ $b = v * t_{res} * SF$=0.332 $\frac{m}{h}$* 4.6 h* 3.5= 5.3 m wide