PET565 PART B: ASSIGNMENT 1

Information

The assignments give you an indication about the main theory and exercises you should be in control of. The total number of points can be used to calculate your grade. 40% correct is required to pass an exam (grade E). 90% is required to get A. You can of course work together and ask for help, but to be given feedback the assignment must be handed in within the deadline 23 March 2018. The assignment is not mandatory to pass the course.

1. Theory (40p)

- State the law of mass action. (5p)
- Define molality and molarity. Show how to calculate one from the other. (5p)
- Define the activity for aqueous, gaseous, surface and mineral species and water. (5p)
- What two classes of equations are used to determine the composition of a system? Which properties are assumed to be conserved? (5p)
- Using van't Hofs law: How does solubility change with temperature for an exotherm reaction? And for an endotherm reaction? (5p)
- Define Ficks laws mathematically. (5p)
- What is the difference between diffusion and dispersion? How are they related? (5p)
- Define the mechanisms and assumptions in the retardation model. (5p)

2. Calculations (55 p)

2.1. **Equilibrium calculations (35 p).** 0.3 mol CaCl2 and 0.05 mol Na2SO4 are mixed into 1 L water.

- Calculate the total concentration C_i of Ca, Cl, Na and SO4.
  Calculate the ionic strength of the brine.
  Calculate and the activity coefficients of the 4 ions (PS: which correlation should be applied?). (5p)
- Assume the complex $CaSO_4^0$ can form with a dissociation constant $K = 10^{-2.5}$.
  Write the dissociation reaction and the corresponding EQ equation.
  Write mass balance equations for Ca and SO4. (5p)
- Find the composition of the brine in terms of m_i, n_i. (5p)

The brine is in equilibrium with a mineral surface that can exchange Ca and Na.

- Define the relevant exchange reaction, equilibrium equation and its constant (see Table 6.4). (5p)
- Assume the Gaines-Thomas convention is used. Calculate the surface composition in terms of β_i. (5p)
- Calculate the composition in terms of β_i^M. (5p)
- Calculate the equilibrium constant based on the brine/surface composition if the Vanselow convention is used (assumes $[i] = \beta_i^M$ for surface species). (5p)

2.2. **Retardation model (20 p).** Consider sorption of a species according to $q = c^2$ where q and c have units mol/L. Water flows with velocity 10 cm/d and the system is 20 cm in length.

- The initial and injected concentrations are $c_0 = 0, c_{inj} = 1$ mol/L. Calculate and plot:
  - the spatial concentration profile along the system after 1 day and 2 days. (5p)
  - the effluent concentration from 0 to 4 d. (5p)
- Now assume the initial and injected concentrations are $c_0 = 1, c_{inj} = 0$ mol/L. Calculate and plot:

- the spatial concentration profile along the system after 1 day and 2 days. (5p)
- the effluent concentration from 0 to 4 d. (5p)