PET565 PART B: EXERCISE SET 3

Goals

- Calculate surface activities of species and compositions.
- Be familiar with some adsorption isotherms and their application.

Important notes

- Assume the activity of surface species is given by equivalent fraction, β_i (Gaines-Thomas convention).

1. Exercises

1.1. Assume a surface storing cations is in equilibrium with a brine containing $m_{\mathrm{Na}^{2+}} = 2, m_{\mathrm{K}^+} = 0.5, m_{\mathrm{Ca}^{2+}} = 0.2$mmol/L. Assume the activity coefficients are 1.

- Write the relevant equilibrium and mass balance equations for this system. Table parameters can be found in the book.
- Calculate the composition of the surface represented by equivalent fractions $\beta_{\mathrm{Na}^{2+}}, \beta_{\mathrm{K}^+}, \beta_{\mathrm{Ca}^{2+}}$. The Gaines-Thomas convention should be applied.
- Derive mathematically, the relation between equivalent fraction composition and the composition in terms of molar fractions.
- From the previous answers, calculate the surface composition in terms of molar fractions $\beta^M_{\mathrm{Na}^{2+}}, \beta^M_{\mathrm{K}^+}, \beta^M_{\mathrm{Ca}^{2+}}$.

1.2. The Langmuir isotherm for adsorption of the species I can be written in the form

$$s_I(c) = s_{\max}\frac{rc_I}{1 + rc_I} \tag{1}$$

where s_I is adsorbed amount in mol/L and c_I is the brine concentration in mol/L.

- Show that the isotherm function is linear for small concentrations.
- Calculate the distribution coefficient as function of brine concentration.
- Show that the isotherm function does not exceed $s_{\max}$.
- We want to ensure that less than 3 mol / L adsorbs. Assume that $s_{\max}$=10mol/L and $r = 1.5[L/mol]$. What is the maximum concentration we can inject?

1.3. A species adsorbs according to a Langmuir isotherm with parameters $s_{\max}$=6mol/L pore and $r = 1.5$ [L/mol].

The species is injected at a concentration of 10 mol/L and a speed of 1 m/min through a porous medium. The initial concentration is 2 mol/L. Consider the state after 1 min injection.

- Calculate the position of the water front, x_w.
- For the concentrations $c = 2, 6, 10$ calculate the retardation factor R and the distance travelled by each concentration. What type of front is observed?
- Plot brine concentration $c(x)$ from $x = 0$ until the water front position.
- Plot adsorbed concentration $q(x)$ from $x = 0$ until the water front position.
- Consider the point $x = 0.5$. Plot the brine concentration at this point as function of time from $t = 0$ to 1 min.
- Repeat the calculations if the initial concentration is $c_0 = 10$mol/L and the injected concentration is 2mol/L.