ChEn 3603 Homework 4

Problem 1 (8 pts)

Beginning with the definition of the total molar flux for species "A" in a binary system

$$N_A = x_A \left(N_A + N_B\right) + J_A \tag{1}$$

1. (4 pts) Derive the expression for the molar flow rate when we have diffusion between concentric spheres but no bulk flow:

   $$n_A = -4\pi r_1 r_2 D_{AB} \left(\frac{c_{A_2} - c_{A_1}}{r_2 - r_1}\right) \tag{2}$$

   You might want to look up in a calculus book or on wikipedia how ∇ is defined in spherical coordinates.

2. (4 pts) Show that $N_A = -\frac{D_{AB} r_1 r_2}{r^2} \frac{c_{A_2} - c_{A_1}}{r_2 - r_1}$ and also derive $N_B(r)$. Justify how you obtain the form for N_B.

Problem 2 (4 pts)

Consider a one-dimensional, binary system of A and B in answering the questions below.

1. (2 pts) For each of the following profiles for J_A, describe the expected profile for $x_A(z)$.
   (a) J_A is a negative constant.
   (b) J_A is linear with positive slope
2. (2 pts) For each of the following profiles for x_A, describe the expected profile for J_A.
   (a) A linear function with negative slope.
   (b) A gaussian function centered at $z = -2$.

Problem 3 (12 pts)

Consider the problem described in SHR 3.5:

> Two bulbs are connected by a tube that is 2 mm in diameter and 10 cm long. Bulb 1 contains argon, and bulb 2 contains xenon. The pressure and temperature are maintained at 1 atm and 105 °C. The binary diffusivity is 0.180 $\mathrm{cm^2/s}$. At time $t = 0$, diffusion begins for argon and xenon between the two bulbs.

Assume that the bulbs have a diameter of 15 cm. Then answer the following questions:

1. (4 pts) determine:
   (a) the time at which the argon mole fraction in the left bulb is 0.7
   (b) the time when the argon mole fraction in the right bulb is 0.25.

   Report these in *hours*.

2. (2 pts) After 75 hours, determine the *molar flux* of both argon and xenon. Report these in $\mathrm{mol}/\mathrm{cm}^2\cdot\mathrm{s}$.
3. (3 pts) After 75 hours, plot the argon and xenon *velocities*, and report the value of v_{argon} and v_{xenon} at $z = L$.
4. (1 pts) After 75 hours, determine the *molar*-averaged velocity of the mixture at $z = L$.
5. (3 pts) After 75 hours, plot the *mass*-averaged velocity of the mixture in the tube and report its value at $z = L$.

Problem 4 (14 pts)

Consider the beaker problem discussed in Example 3.2 in SHR where benzene is evaporating into air. Let's estimate how long it will take the benzene to evaporate completely from the beaker in two different ways:

1. (8 pts) Assume that N_A is constant in time and can be evaluated at $t = 0$.
2. (6 pts) Account for the variation in N_A with the liquid level.

Compare these results. Which do you think should be more accurate? Why?

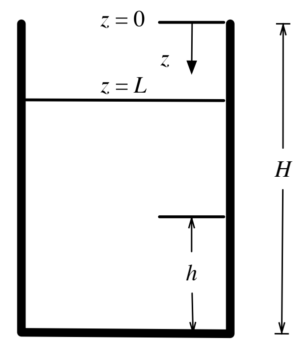

Figure 1: The beaker, showing the coordinate system and definitions of L, h and H.

Additional information

In solving this problem, use the following:

- Raoult's law with the Antoine equation to determine the vapor phase composition of benzene at the vapor-liquid interface. You can find Antoine equation parameters for *many* substances from the NIST Webbook.
- Pseudo-steady state assumption to allow us to determine N_A assuming a fixed liquid interface.
- Start with a mole balance on benzene in the *liquid phase* using the equation we developed in class:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathsf{V}_{(t)}} c_i \,\mathrm{dV} = -\int_{\mathsf{S}_{(t)}} \mathbf{N}_i \cdot \mathbf{a}\,\mathrm{dS} + \int_{\mathsf{V}_{(t)}} S_i \,\mathrm{dV} \tag{3}$$

- Be careful since you will end up with c in the gas phase and c in the liquid phase. These are very different. I suggest that you call the liquid phase molar concentration c^ℓ to keep your sanity.

Hint:

Note that $h = H - z$ so that $dh = -dz$ and $z = [L, H]$ (starts at L and ends at H when the beaker runs dry). This should help with the left-hand-side of (3).