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Exercise 4: TMT4208

Hand out: 01.02.2021
Seminar: 05.02.2021
Hand in: 12.02.2021

Task 1: Diffusion through a stagnant gas (Stefan diffusion)

In this task we will consider a tube with a liquid consisting of specie A which is evaporating into a gas phase which contains species A and B - where the latter is insoluble in the liquid. A sketch of the system is shown in figure 1a.

The system is considered as 1D with the liquid interface at $z = z_1$, where the mole fraction of A in the gas is X_{A1}. At the top of the tube, $z = z_2$, the concentration is X_{A2}. The concentrations are assumed constant and phase B is considered stagnant.

a. Fick's first law for component A in the gas phase is expressed as:

$$\dot{\boldsymbol{n}}_A = -\mathcal{C}\mathcal{D}\nabla X_A + \mathcal{C}\tilde{\boldsymbol{u}}X_A \tag{1}$$

what is the significance of each of the terms and the interpretation of the velocity $\tilde{\boldsymbol{u}}$? Under what conditions is this velocity equivalent to the normal (mass based) velocity $\boldsymbol{u}$?

b. Show that the above equation reduces to

$$\dot{n}_A = -\frac{\mathcal{C}\mathcal{D}}{1 - X_A}\frac{\partial X_A}{\partial z} \tag{2}$$

when assuming 1D flow and stagnant B.

c. Under steady state conditions, it can be shown that the molar flux of A is constant. Demonstrate that this is the case and show that the final governing equation for the mole fraction can be written as:

$$\frac{\partial}{\partial z}\left(\frac{\mathcal{C}\mathcal{D}}{1 - X_A}\frac{\partial X_A}{\partial z}\right) = 0 \tag{3}$$

d. Assuming that $\mathcal{C}$ and $\mathcal{D}$ are constant, show that the mole fraction of A can be written as:

$$\left(\frac{1 - X_A}{1 - X_{A1}}\right) = \left(\frac{1 - X_{A2}}{1 - X_{A1}}\right)^{\frac{z - z_1}{z_2 - z_1}} \tag{4}$$

Hint: Using $z_1 = 0$ and $z_2 - z_1 = L$ simplifies the task.

Task 2: Concentration equalization by diffusion

In this task, we will consider concentration equalization in a gas mixture present in a system as sketched in figure 1b. The system is characterized by two containers, α and β, each of which have a volume $V = 1.0$ liter, (total) pressure 1 bar and temperature 300 K, which are connected by a capillary tube of length L=20 mm and cross sectional area $a = 1.5$ mm^2. The diffusivity of the binary gas mixture is assumed to be constant and equal to $\mathcal{D} = 0.78 \cdot 10^{-4}$ m^2/s and each of the species (and the resulting mixture as well) is assumed to behave as an ideal gas. Initially, that is at $t = 0$, container α contains pure A and container β contains pure B.

a. Show that there only is a single diffusion coefficient in binary mixtures - i.e. that $\mathcal{D}_{AB} = \mathcal{D}_{BA} = \mathcal{D}$.

b. Why will the system described in this task result in equimolar counter diffusion?

c. Assuming so called quasi-stationary conditions, that is $\dot{n}_A$=constant, show that

$$\dot{n}_A = \frac{\mathcal{C}\mathcal{D}}{L}\left(X_{A\alpha} - X_{A\beta}\right), \tag{5}$$

where $X_{A\alpha}$ and $X_{A\beta}$ signify the mole fractions of specie A in containers α and β, respectively.

d. Determine the *half-time* of the concentration difference $\Delta X_A = X_{A\alpha} - X_{A\beta}$, i.e. the time required to reach $\Delta X_A = 0.5$, corresponding to $X_{A\alpha} = 0.75$ and $X_{A\beta} = 0.25$.

Hint: Consider each of the containers α and β as systems which respectively are losing and gaining specie A at a constant rate $\pm a\dot{n}_A$ [mol/s].

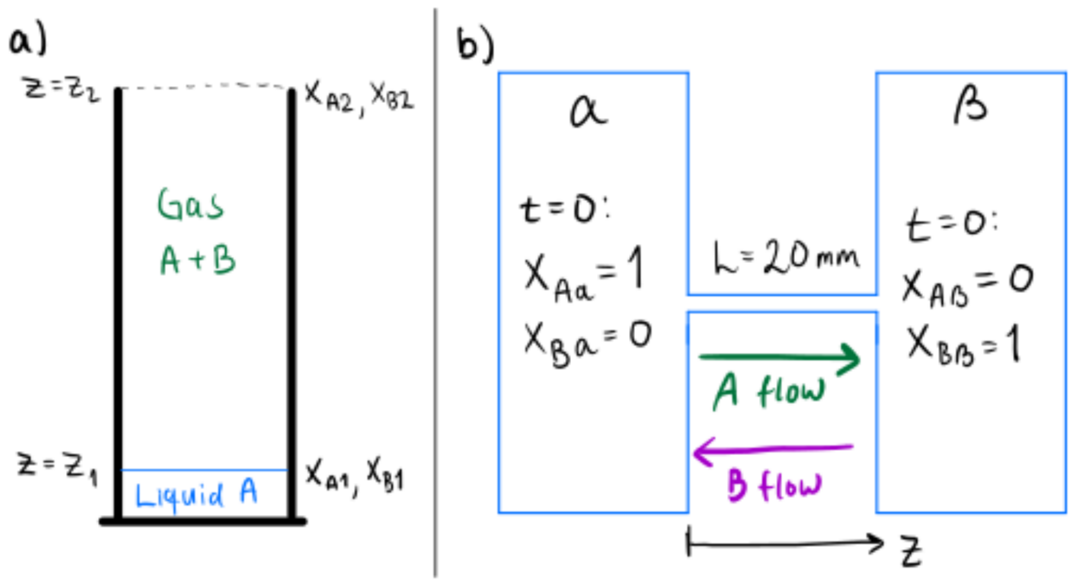

Figure 1: Two different diffusive systems.