Two-bulb dynamic diffusion experiment

March 17, 2022

Introduction

Simulation of the three-component two-bulb diffusion experiment. The experiment consists of two small compartments connected by a tube through which the components can diffuse. The three components considered here are H_2, N_2 and CO_2. The Maxwell-Stefan equations are used to model diffusion.

Model equations

The Maxwell-Stefan equations are:

$$-\frac{x_i}{RT}\nabla\mu_i = \sum_{j\neq i}\frac{x_j\mathbf{J}_i - x_i\mathbf{J}_j}{c_t D_{ij}} \tag{1}$$

The left side of (1) can be reformulated, giving:

$$-\left(\frac{\partial \ln \gamma_i}{\partial \ln x_i} + 1\right)\nabla x_i = \sum_{j\neq i}\frac{x_j\mathbf{J}_i - x_i\mathbf{J}_j}{c_t D_{ij}} \tag{2}$$

For ideal systems the activity coefficient γ_i of component i is equal to unity. The left side of (2) then simplifies, resulting in:

$$-\nabla x_i = \sum_{j\neq i}\frac{x_j\mathbf{J}_i - x_i\mathbf{J}_j}{c_t D_{ij}} \tag{3}$$

The change in local composition at any given time is:

$$c_t\frac{\partial x_i}{\partial t} = -\nabla\cdot\mathbf{J}_i \tag{4}$$

To preserve the total concentration the fluxes of the different components sum up to zero:

$$\sum_i \mathbf{J}_i = 0 \tag{5}$$

Method

The mole fractions of H_2, N_2 and CO_2 in the first compartment are initially 0.0, 0.501 and 0.499, respectively. In the second compartment the mole fractions of H_2, N_2 and CO_2 are initially 0.501, 0.499 and 0.0, respectively. The diffusivities are $D_{12} = 8.33e-5$ (m^2/s), $D_{13} = 6.8e-5$ (m^2/s) and $D_{23} = 1.68e-5$ (m^2/s). The volumes of the compartments are $5e-4$ (m^3) and the tube connecting the compartments has a length of $1e-2$ (m) and a diameter of $2e-3$ (m).

To simulate the transient two-bulb diffusion experiment, the model equations are solved. This is done by first computing the fluxes with (3), given some composition. Then, the fluxes are used to update the composition with (4). Results are shown in figure 1.

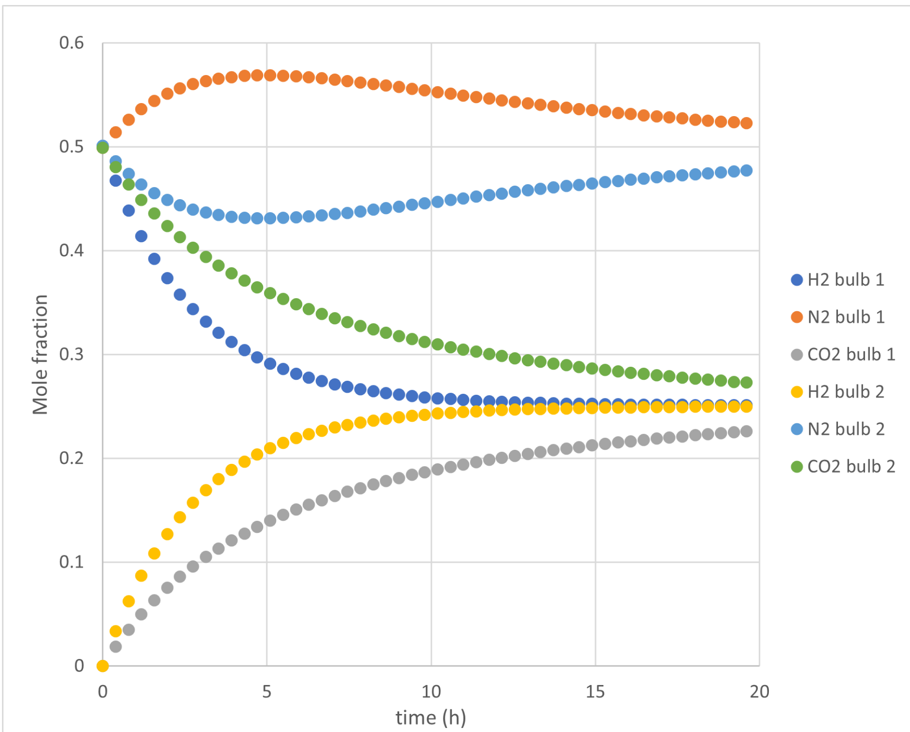

Figure 1: The mole fraction as a function of time (h).

Appendix

Here the one-dimensional case of the Maxwell-Stefan equations modeling the two-bulb diffusion experiment is elaborated on. The local fluxes are computed by solving the linear system representing (3):

$$A\mathbf{J} = \mathbf{b} \tag{6}$$

With A, $\mathbf{J}$ and $\mathbf{b}$ given by:

$$A = (a_{ij}) \tag{7}$$

$$\mathbf{J} = (J_i) \tag{8}$$

$$\mathbf{b} = \left(-c_t \frac{\partial x_i}{\partial z}\right) \tag{9}$$

The elements of A are:

$$a_{ij} = \frac{x_i}{D_{in}} + \sum_{j \neq i} \frac{x_j}{D_{ij}} \qquad i = j \tag{10}$$

$$a_{ij} = -x_i \left(\frac{1}{D_{ij}} - \frac{1}{D_{in}}\right) \qquad i \neq j \tag{11}$$