Two-bulb diffusion experiment

March 16, 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. These are solved using the finite volume method. Time discretization is fully implicit. Results are shown in figure 1.

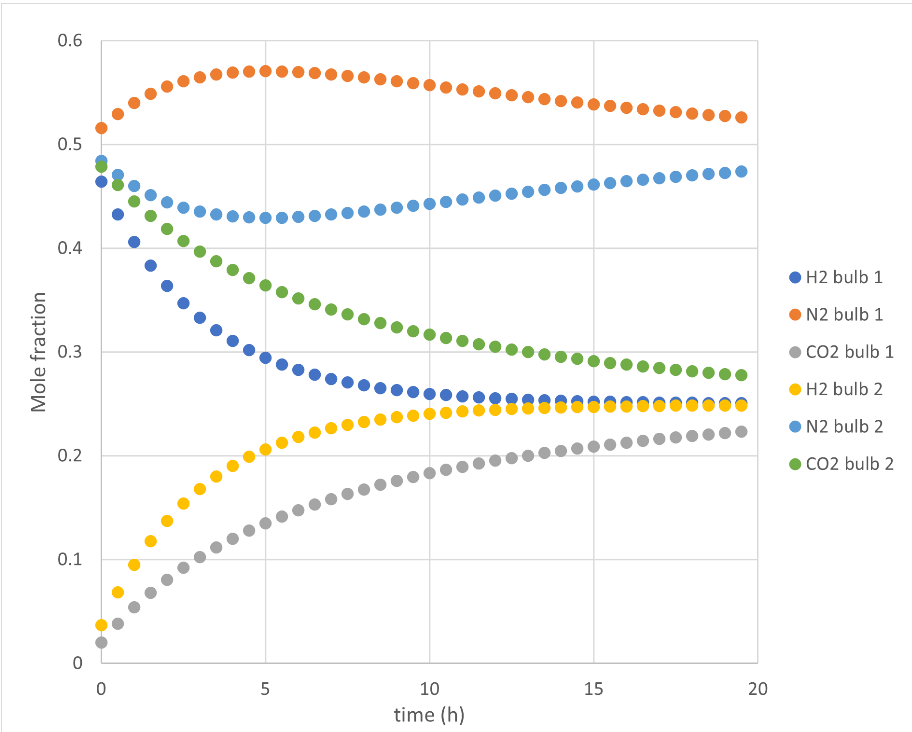

Figure 1: The mole fraction as a function of time (h).

Appendix

Here the one-dimensional case of the Maxwell-Stefan equations, applicable to the three-component two-bulb diffusion experiment, is elaborated on. The one-dimensional case of (3) for component 1 is:

$$-c_t \frac{\partial x_1}{\partial z} = \frac{x_2 J_1 - x_1 J_2}{D_{12}} + \frac{x_3 J_1 - x_1 J_3}{D_{13}} \tag{6}$$

The equation for component 2 is:

$$-c_t \frac{\partial x_2}{\partial z} = \frac{x_1 J_2 - x_2 J_1}{D_{12}} + \frac{x_3 J_2 - x_2 J_3}{D_{23}} \tag{7}$$

The change in local composition of component 1 is:

$$c_t \frac{\partial x_1}{\partial t} = -\frac{\partial J_1}{\partial z} \tag{8}$$

The change in local composition of component 2 is:

$$c_t \frac{\partial x_2}{\partial t} = -\frac{\partial J_2}{\partial z} \tag{9}$$

To facilitate the elimination of the fluxes from the equations above equation (6) and (7) are rewritten:

$$-c_t \frac{\partial x_1}{\partial z} = a_1 J_1 + a_2 J_2 \tag{10}$$

$$-c_t \frac{\partial x_2}{\partial z} = b_1 J_1 + b_2 J_2 \tag{11}$$

With a_1, a_2, b_1 and b_2 given by:

$$a_1 = \left(\frac{1}{D_{12}} - \frac{1}{D_{13}}\right) x_2 + \frac{1}{D_{13}} \tag{12}$$

$$a_2 = x_1 \left(\frac{1}{D_{13}} - \frac{1}{D_{12}}\right) \tag{13}$$

$$b_1 = x_2 \left(\frac{1}{D_{23}} - \frac{1}{D_{12}}\right) \tag{14}$$

$$b_2 = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}}\right) x_1 + \frac{1}{D_{23}} \tag{15}$$

The fluxes can now be written in terms of the composition gradients:

$$J_1 = \beta_1 \frac{\partial x_1}{\partial z} + \beta_2 \frac{\partial x_2}{\partial z} \tag{16}$$

$$J_2 = \alpha_1 \frac{\partial x_1}{\partial z} + \alpha_2 \frac{\partial x_2}{\partial z} \tag{17}$$

With β_1, β_2, α_1 and α_2 given by:

$$\beta_1 = -\frac{c_t}{a_1} - \frac{a_2\alpha_1}{a_1} \tag{18}$$

$$\beta_2 = -\frac{a_2\alpha_2}{a_1} \tag{19}$$

$$\alpha_1 = -\frac{c_t}{\left(a_2 - \frac{a_1 b_2}{b_1}\right)} \tag{20}$$

$$\alpha_2 = \frac{a_1 c_t}{(a_2 b_1 - a_1 b_2)} \tag{21}$$

Equations (16) and (17), together with (8) and (9) are the set of equations which are solved to simulate three-component two-bulb diffusion.