Two-bulb diffusion experiment

March 14, 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:

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

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.

Appendix

Here the one-dimensional case of the Maxwell-Stefan equations, applicable to the three-component two-bulb diffusion experiment. The one-dimensional case

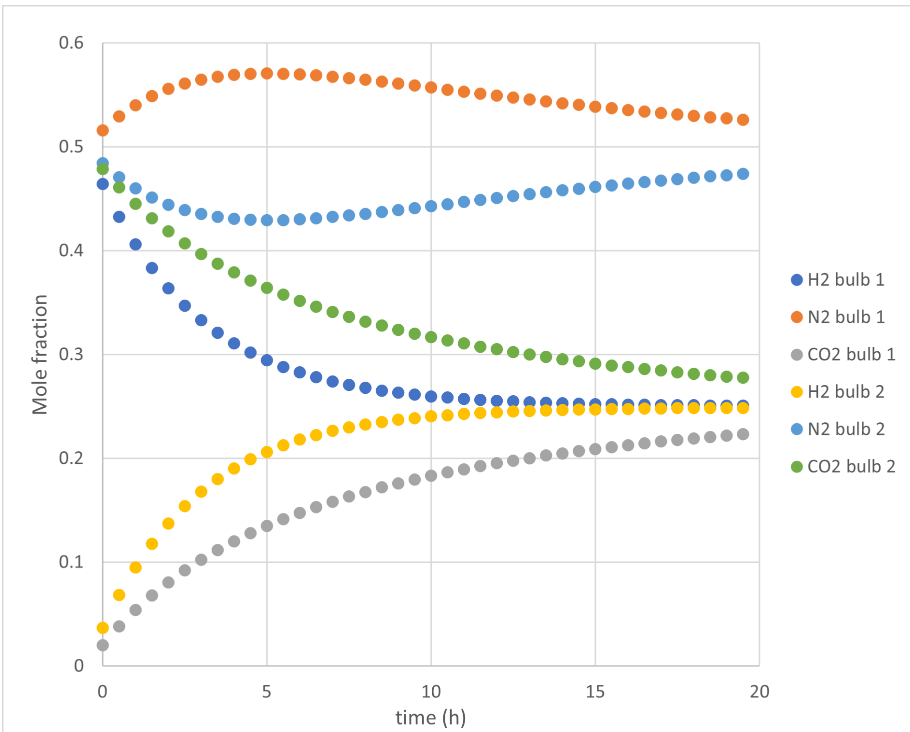

Figure 1: The mole fraction as a function of time (h).

of (3) for component 1 is:

$$-c_t \frac{\partial x_1}{\partial z} = \frac{x_2 J_1 - x_1 J_2}{D_{12}} + \frac{x_3 J_1 - x_1 J_3}{D_{13}} \tag{5}$$

The equation for component 2 is:

$$-c_t \frac{\partial x_2}{\partial z} = \frac{x_1 J_2 - x_2 J_1}{D_{12}} + \frac{x_3 J_2 - x_2 J_3}{D_{23}} \tag{6}$$

The change in local composition of component 1 is:

$$c_t \frac{\partial x_1}{\partial t} = -\frac{\partial J_1}{\partial z} \tag{7}$$

The change in local composition of component 2 is:

$$c_t \frac{\partial x_2}{\partial t} = -\frac{\partial J_2}{\partial z} \tag{8}$$

To facilitate the elimination of the fluxes from the equations above equation (5) and (6) are rewritten:

$$-c_t \frac{\partial x_1}{\partial z} = a_1 J_1 + a_2 J_2 \tag{9}$$

$$-c_t \frac{\partial x_2}{\partial z} = b_1 J_1 + b_2 J_2 \tag{10}$$

With a_1, a_2, b_1 and b_2 given by:

$$a_1 = \left(\frac{1}{D_{12}} - \frac{1}{D_{13}}\right) x_2 + v_1 \tag{11}$$

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

$$b_1 = x_2 \left(\frac{1}{D_{23}} - \frac{1}{D_{12}}\right) \tag{13}$$

$$b_2 = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}}\right) x_1 + v_3 \tag{14}$$

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

$$J_1 = \beta_1 \frac{\partial x_1}{\partial z} + \beta_2 \frac{\partial x_2}{\partial z} \tag{15}$$

$$J_2 = \alpha_1 \frac{\partial x_1}{\partial z} + \alpha_2 \frac{\partial x_2}{\partial z} \tag{16}$$

With β_1, β_2, α_1 and α_2 given by:

$$\beta_1 = -\frac{c_t}{a_1} - \frac{a_2 \alpha_1}{a_1} \tag{17}$$

$$\beta_2 = -\frac{a_2 \alpha_2}{a_1} \tag{18}$$

$$\alpha_1 = -\frac{c_t}{\left(a_2 - \frac{a_1 b_2}{b_1}\right)} \tag{19}$$

$$\alpha_2 = \frac{a_1 c_t}{(a_2 b_1 - a_1 b_2)} \tag{20}$$

Equations (15) and (16), together with (7) and (8) are the set of equations which are solved to simulate three-component two-bulb diffusion.