Two-bulb dynamic diffusion experiment

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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. The equations are solved by first computing the fluxes, given some composition. The computed fluxes are then used to update the composition.

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 mole fraction at a given time is:

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

Results

The Maxwell-Stefan equations were solved to simulate diffusion in the two-bulb, three-component system. The mole fractions of H_2, N_2 and CO_2 in the first compartment were initially 0.0, 0.501 and 0.499, respectively. In the second compartment the mole fractions of H_2, N_2 and CO_2 were initially 0.501, 0.499 and 0.0, respectively. The diffusivities were $D_{12} = 8.33e-5$ (m^2/s), $D_{13} = 6.8e-5$ (m^2/s) and $D_{23} = 1.68e-5$ (m^2/s). The volume of the compartments were $5e-4$ (m^3) and the tube connecting the compartments had a length of $1e-2$ (m) and a diameter of $2e-3$ (m). Results are shown in figure 1.

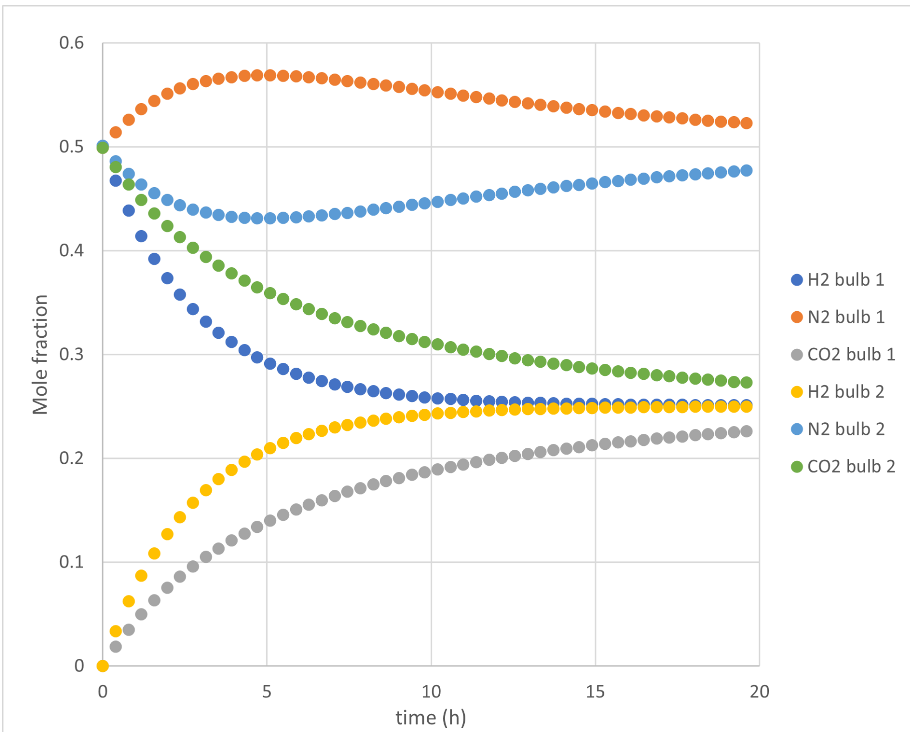

Figure 1: The mole fraction as a function of time (h).