

Two-bulb 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. These equations are solved using a dynamic multi-directional search.

Model equations

The Maxwell-Stefan equations are:

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

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

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

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

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

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.

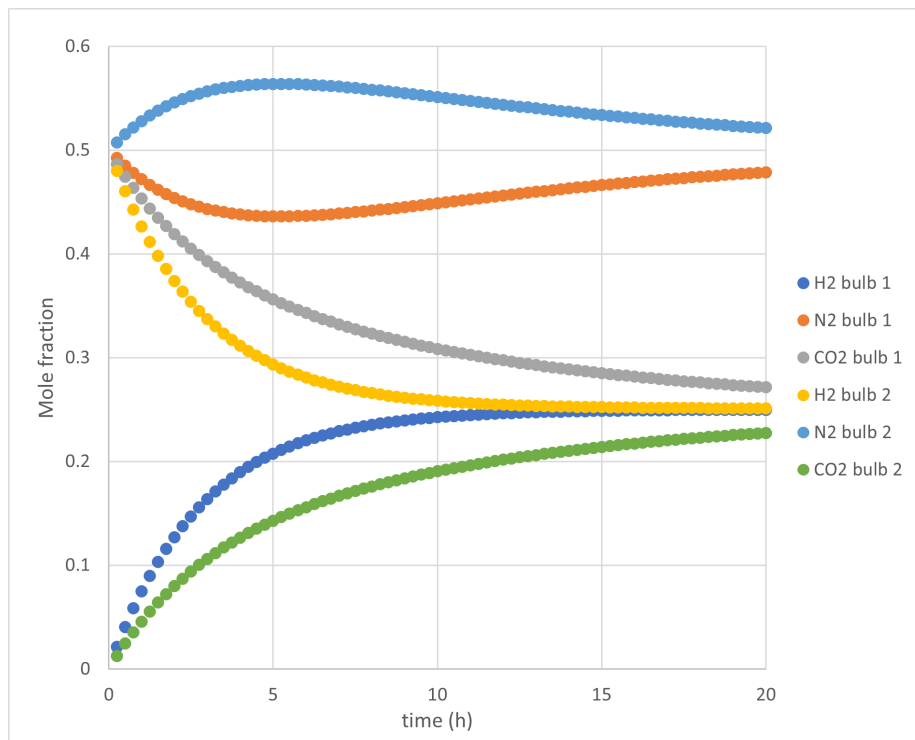


Figure 1: The mole fraction as a function of time (h).