Two-bulb diffusion experiment

Derek W. Harrison

March 6, 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:

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

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

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

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

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

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 the diameter was $2e-3$ (m). Results are shown in figure 1,

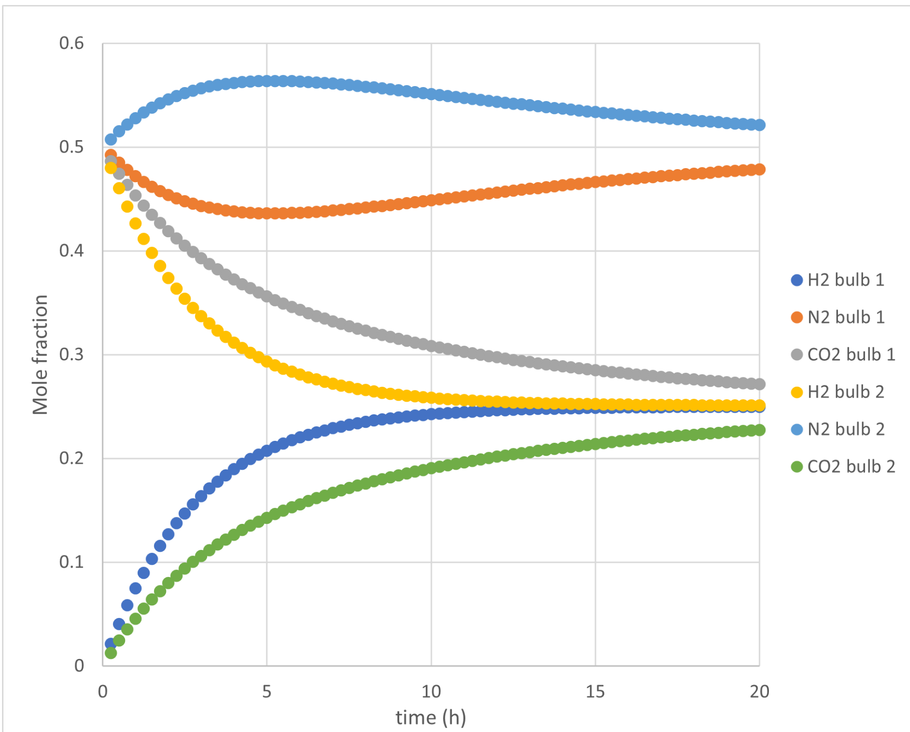

Figure 1: The mole fraction as a function of time (h).