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.

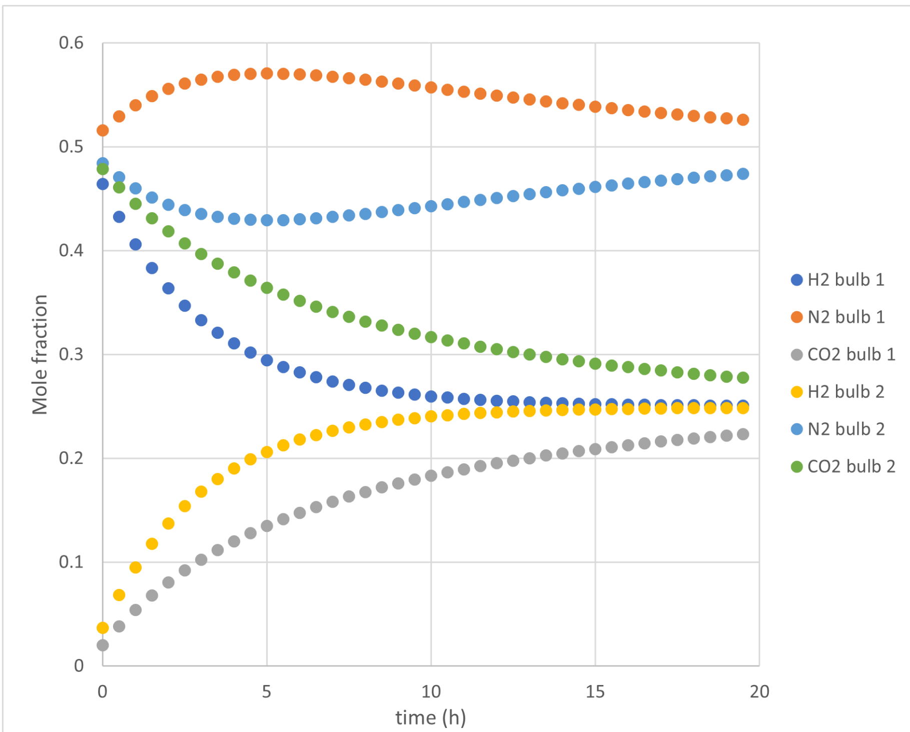

Figure 1: The mole fraction as a function of time (h).