ChE 548
Final Exam
May 8, 2007

Problem 1. Consider an ideal gas binary mixture under isothermal conditions flowing down a pipe. The total mass balance, composition balance, and momentum balance are respectively,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) \tag{1}$$

$$\rho \frac{\partial w_A}{\partial t} = -\rho \mathbf{v} \cdot \nabla w_A - \nabla \cdot \mathbf{j}_A \tag{2}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla(\mathbf{v}) - \nabla p - \nabla \cdot \tau - \rho \nabla \hat{\Phi} \quad , \tag{3}$$

where ρ is the mass density, w_A is the mass fraction of component A, and **v** is the center-of-mass velocity. The necessary constitutive equations to define this system are the ideal gas equation, Fick's Law, and Newton's law of viscosity.

$$\mathbf{j}_A = -\rho D \nabla w_A \tag{4}$$

$$p = \frac{N}{V} RT = \left(\frac{w_A}{m_A} + \frac{w_B}{m_B} \right) \rho RT = \left(\frac{1}{m_B} + \frac{m_B - m_A}{m_B m_A} w_A \right) \rho RT \tag{5}$$

$$\tau_{ij} = -\mu \left(\frac{\partial v_j}{\partial z_i} + \frac{\partial v_i}{\partial z_j} \right) + \left(\frac{2}{3}\mu - \kappa \right) \sum_{i=1}^{3} \frac{\partial v_i}{\partial z_i} \delta_{ij} \tag{6}$$

where D is the diffusivity, R is the gas constant, T is the temperature, m_A and m_B are the molecular weights, μ is the shear viscosity and κ is the bulk viscosity.

Assume there is no external potential, $\hat{\Phi}$. Assume the system is at steady state. Assume there is flow only in the z-dimension (axial dimension) and that there is no dependence of the properties on the radial or angular dimensions. (In this case, only the zz component of the extra stress tensor, τ, is relevant.) Assume further that the transport properties constant.

(a) Write the simplified mass and momentum balances, equations (1) through (3) for the assumptions given above. Substitute equations (4) through (6) into your solution.
(b) Define a set of dimensionless variables as follows:

$$y = \begin{bmatrix} \frac{\rho}{\rho_s} & \frac{1}{\rho_s}\frac{\partial \rho}{\partial \zeta} & \frac{w_A}{w_{A,s}} & \frac{1}{w_{A,s}}\frac{\partial w_A}{\partial \zeta} & \frac{1}{v_{z,s}} v_z & \frac{1}{v_{z,s}}\frac{\partial v_z}{\partial \zeta} \end{bmatrix}^T , \tag{7}$$

Write dimensionless evolution equations for each of these six dimensionless variables.
(c) Indicate the dimensionless constants that result as a consequence of your procedure for making the equations dimensionless in part (b). Explain the meaning of each of the dimensionless variables.

Problem 2.
Explain with texts and accompanying sketches how one determines if a molecular dynamics simulation has been run long enough to obtain a reliable self-diffusivity. What will you expect if you have not run the simulation long enough? Given the same temperature, should you have to run longer for a liquid or gas?

solution:

Plot the mean square displacement as a function of time on a log-log plot. compute the exponent. The exponent will be unity if you have reached the long-time limit required by the Einstein relation for the self-diffusivity.

If you haven't run the simulation long enough, the exponent will be between 1 and 2.

You need to run longer for a gas because the time between collisions is longer in a gas.

Solutions:

Problem 1.

(a) Write the simplified mass and momentum balances, equations (1) through (3) for the assumptions given above. Substitute equations (4) through (6) into your solution.

$$0 = \frac{\partial \rho v_z}{\partial z} \quad , \tag{II.1.a}$$

$$0 = -\rho v_z \frac{\partial w_A}{\partial z} + \frac{\partial}{\partial z}\left(\rho D \frac{\partial w_A}{\partial z} \right) \quad , \tag{II.1.b}$$

$$0 = -\rho v_z \frac{\partial v_z}{\partial z} - \frac{\partial p}{\partial z} - \frac{\partial \tau_{zz}}{\partial z} \tag{II.1.c}$$

The required derivatives of the constitutive equations in the momentum balance are

$$\frac{\partial p}{\partial z} = RT\left(\left(\frac{1}{m_B} + \frac{m_B - m_A}{m_B m_A} w_A \right) \frac{\partial \rho}{\partial z} + \rho \frac{m_B - m_A}{m_B m_A} \frac{\partial w_A}{\partial z} \right) \quad . \tag{II.2}$$

For the extra stress tensor, the convention that we follow for Newton's law of viscosity defines the two viscosities in relation to the viscous stresses as [1-3]

$$\frac{\partial \tau_{zz}}{\partial z} = -\frac{\partial}{\partial z}\left(\frac{4}{3}\mu + \kappa \right) \cdot \frac{\partial v_z}{\partial z} - \left(\frac{4}{3}\mu + \kappa \right) \frac{\partial^2 v_z}{\partial z^2} \quad . \tag{II.3}$$

(b) Write dimensionless evolution equations for each of these six dimensionless variables.

$$\frac{\partial y_1}{\partial \zeta} = y_2 \tag{II.5.a}$$

$$y_2 = -\frac{y_1 y_6}{y_5} \tag{II.5.b}$$

$$\frac{\partial y_3}{\partial \zeta} = y_4 \tag{II.5.c}$$

$$\frac{\partial y_4}{\partial \zeta} = N_{Pe} y_4 y_5 - \frac{y_2 y_4}{y_1} \tag{II.5.d}$$

$$\frac{\partial y_5}{\partial \zeta} = y_6 \qquad \text{(II.5.e)}$$

$$\frac{\partial y_6}{\partial \zeta} = N_{\text{Re}} y_1 y_5 y_6 + N_{\text{Re}} N_T \left(\frac{1}{N_{AB}} y_2 + N_w y_3 y_2 - N_w y_1 y_4 \right) \qquad \text{(II.5.f)}$$

(c) Indicate the dimensionless constants that result as a consequence of your procedure for making the equations dimensionless in part (b). Explain the meaning of each of the dimensionless variables.

We have introduced five dimensionless variables: the Péclet number (ratio of convective to diffusive forces), the Reynolds number (ratio of convective to viscous forces), a ratio of molecular weights, a dimensionless temperature and a composition ratio, given respectively by

$$N_{Pe} = \frac{L v_{z,s}}{D} \qquad \text{(II.6.a)}$$

$$N_{\text{Re}} = \frac{L \rho_s v_{z,s}}{\left(\frac{4}{3}\mu + \kappa \right)} \qquad \text{(II.6.b)}$$

$$N_{AB} = \frac{m_A}{m_B} \qquad \text{(II.6.c)}$$

$$N_T = \frac{RT}{m_A v_{z,s}^2} \qquad \text{(II.6.d)}$$

$$N_w = \frac{N_{AB} - 1}{N_{AB}} w_{A,s} \qquad \text{(II.6.e)}$$