CBE 548: Advanced Transport Phenomena II
Spring, 2010
Midterm

Problem 1. Basics of Mass Transfer

Consider diffusion in a binary, isothermal system. One can write Fick's law as

$$\mathbf{j}_A = -\rho D \nabla w_A \qquad \mathbf{j}_B = -\rho D \nabla w_B \tag{1.1}$$

where $\mathbf{j}_A = \rho w_A (\mathbf{v}_A - \mathbf{v})$ and $\mathbf{v} = w_A \mathbf{v}_A + w_B \mathbf{v}_B$.

(a) What three assumptions are implicit in this constitutive equation?

Now consider a different constitutive equation

$$\mathbf{J}^*_\mathbf{A} = -cD^\circ_{AB} \nabla w_A \qquad \mathbf{J}^*_\mathbf{B} = -cD^\circ_{BA} \nabla w_B \tag{1.2}$$

where $\mathbf{J*}_A = cx_A (\mathbf{v}_A - \mathbf{v*})$ and $\mathbf{v*} = x_A \mathbf{v}_A + x_B \mathbf{v}_B$.

(b) What is the relationship between D°_{AB} and D°_{BA}?
(c) What is the relationship between D°_{AB} and D?

Problem 2. Traditional Methods of Estimating Diffusivities

For a single component gas, one can use kinetic theory to estimate the self diffusivity,

$$D_{self,A} = \frac{1}{3} \bar{u} \lambda \tag{2.1}$$

where the mean molecular speed, $\bar{u}$, is

$$\bar{u} = \sqrt{\frac{8 k_B T}{\pi m_A}} \tag{2.2}$$

and where the mean free path, λ, is

$$\lambda = \frac{1}{\sqrt{2} \pi d_A^2 n} \tag{2.3}$$

where k_B is Boltzmann's constant, T is temperature, m_A is the mass of component A, d_A is the collision diameter of component A and n is the number density of component A.

These numbers may be useful:

k_B = 1.38066x10^{-23} J/K/molecule
N_{AV} = 6.02205x10^{23} molecule/mole
R = 8.31441 J/K/mole
1 amu = 1.66056x10^{-27} kg

name	molecular weight	collision diameter (Å)
bromine	159.82	4.268
helium	4.003	2.576

(a) Explain, from a molecular level point of view, the qualitative temperature and density dependence of the self diffusivity.
(b) What is the self-diffusivity of bromine at 400 K and 1 atm?
(c) At the same temperature and density, is the diffusivity of bromine higher or lower than that of helium? Why?
(d) For a 50/50 molar mixture of bromine and helium, use the Darken equation to estimate the Fickian diffusivity at 400 K and 1 atm? Assume ideal gas. He self-diffusivity at these conditions is 8.96x10^{-5} m^2/s.

Problem 3. Generating Transport Properties from Molecular-Level Simulation

In homeworks 2 and 3, you used molecular dynamics simulation to generate self-diffusivities of pure fluids and mixtures in the gas and liquid states.

(a) In your own words, what are the three most significant weaknesses of using molecular simulation to generate transport properties?
(b) What are the three most significant strengths?