ChE 548
Final Exam
May 2, 2008

Problem 1.
Consider the steady state behavior of a three component fluid located in an isothermal and isobaric system between two boundaries. The thermodynamic state of the boundary at z = 0 is defined by the mole fraction of 1, $x_1 = 0.25$, mole fraction of 2, $x_2 = 0.74$, temperature T = 300 K, and pressure p = 1 bar. The thermodynamic state of the boundary at z = 1 m is defined by the mole fraction of 1, $x_1 = 0.2$, mole fraction of 3, $w_3 = 0.79$, temperature T = 300 K, and pressure p = 1 bar.

The chemical potential of component i in a multicomponent van der Waals gas is given by

$$\mu_i = -k_B T \ln\left(\frac{V_m - b_{mix}}{x_i \Lambda_i^3}\right) + \frac{k_B T b_i}{V_m - b_{mix}} - \frac{2}{V_m}\sum_{j=1}^{N_c} x_j a_{ij} \quad (1)$$

where kB is Boltzmann's constant, V_m is the molar volume, Li is the thermal de Broglie wavelength. For this example, we will set all of the van der Waal b parameters (all b_i and b_{mix}) to zero. The values of a are as follows: $a_{11} = a_{22} = a_{33} = a_{13} = a_{23} = a_{31} = a_{32} = 0$, $a_{12} = a_{21} = 20$ Joules-m^3/mole. Consider the molar volume to be constant at $V_m = 2.5\text{x}10^{-2}$ m^3/mole.

Tasks.
(a) Using a finite difference formula, determine the average mole fraction gradients for each component, based on the boundary values.
(b) Based on the sign of the mole fraction gradients, in which direction would you expect the diffusive flux of each species to be?
(c) Using a finite difference formula, determine the average chemical potential gradients for each component, based on the boundary values.
(d) Based on the sign of the chemical potential gradients, in which direction would you expect the diffusive flux of each species to be?
(e) Based on your conclusions in parts (b) and (d), which fluxes will one actually observe, those given in part (b) or part (d)? Why?
(f) What is the common term given to the transport phenomena exhibited by one of the components?
(g) Name a chemical engineering unit operation in which this transport phenomena is frequently exploited.

Problem 2.

Consider the driving force for mass flux given in equation (24.1-8) of BSL2 on page 766 and the flux law given in equation (24.2-3) on page 767. Further consider an isothermal, isobaric system in the absence of external forces. Note that the diffusivities that appear in (24.2-3) are symmetric $D_{\alpha\beta} = D_{\beta\alpha}$ and satisfy the constraints $\sum_{\alpha} w_{\alpha} D_{\alpha\beta} = 0$.

(a) How many independent diffusivities are there for a ternary system?
(b) For a ternary system, express the off-diagonal elements of the diffusivity as a function of the diagonal components.
(c) In this formulation, if the diagonal components are constants with respect to composition, are the off-diagonal components also constant with respect to composition.
(d) Consider a ternary system, free of convection at steady state, where the diffusive fluxes are constant. Express each flux in terms of the minimum number of independent driving forces. For simplicity, you may assume that the fluid is an ideal mixture where the activity of component i is equal to the mole fraction of component i.

Problem 3.
Consider the following composition balance

$$\rho \frac{\partial w_A}{\partial t} = -\rho \mathbf{v} \cdot \nabla w_A - \nabla \cdot \mathbf{j}_A + \sum_{i=1}^{N_R} r_{i,A} \quad , \tag{14}$$

where the diffusive mass flux of component A relative to the center of mass velocity is defined as

$$\mathbf{j}_A = -\rho D \nabla w_A \cdot \quad , \tag{15}$$

and there is one chemical reaction in the system ($N_R = 1$) with a rate given by

$$r_A = -k\rho_A \quad , \tag{16}$$

Put this equation in dimensionless form. Identify all dimensionless numbers.