ChE 548: Advanced Transport Phenomena II
Department of Chemical Engineering, University of Tennessee, Knoxville
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Midterm Examination
Administered: March 19, 2004

Problem 1.
Consider an isothermal binary mixture of A and B with molecular weights, M_A and M_B, at a thermodynamic state specified by density, ρ, temperature, T, and mass fraction, w_A. We experimentally measure the average velocity of component A and component B along the axis of a cylindrical tube relative to laboratory frame of reference, v_A and v_B, which are constant over the length of the cylinder. Answer the following questions. Assume we choose to measure diffusion relative to the center of mass velocity. Also assume that we will use a form of Fick's law that gives mass flux as a function of gradient in mass fraction.

a. What is the center of mass velocity, v, in this system?
b. What is the total flux of component A in this system?
c. What is the convective flux of component A in this system?
d. What is the diffusive flux of component A in this system, given in terms of the variables listed in the problem statement? Give it in the most simplified form.
e. What form of Fick's law is appropriate for the assumptions listed in the problem statement?
f. Assuming we know the diffusivity, D, of this system, what is the gradient of the mass fraction of component A in this system?
g. Using symmetry relations, answer parts (d) and (f) for component B.
h. Do your results satisfy that the sum of the diffusive fluxes must be zero? Why or why not?
i. Do your results satisfy the constraint that the gradient of the mass fraction of A must be equal in magnitude and opposite in sign to the gradient of the mass fraction of B?
j. What is the profile of the mass fraction of A along the cylinder axis?

Problem 2.
You have performed a molecular dynamics simulation in the microcanonical ensemble, which maintains a constant number of molecules, N, system volume, V, and total energy, E. You have simulated a relatively dilute gas. You use an initial configuration of a simple cubic lattice. In this initial configuration, there are no molecules within the interaction cut-off distance of each other. You equilibrate using velocity scaling to maintain a constant set temperature for maxeqb steps.

a. What is the initial potential energy?
b. If at the beginning of the data production stage, your temperature increases beyond the set temperature, what is causing the increase?
c. How can you fix this problem?
d. You wanted to simulate at a given pressure (say 10 atm) and temperature. You fed that pressure and temperature into an equation of state, and obtained an estimate of the molar density, N/V. You simulated at that N and V and calculated from the simulation a negative pressure. List and explain with text or plots possible reasons for the negative pressure. What does it mean?