ChE 548
Final Exam
Spring, 2005

Problem 1.
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?

Problem 2.
Consider an incompressible fluid composed of two components A and B. Write out the material, momentum, and energy balances that describe the steady state profile of material under the following boundary conditions.

$$\rho(z=0)=\rho_o$$

$$w_A(z=0)=w_{Ao} \qquad w_A(z=L)=w_{AL}$$

$$v(z=0)=0$$

$$T(z=0)=T_{low} \qquad T(z=L)=T_{high}$$

You will need to invoke Fick's law and Fourier's law. Write out the equations for each of three cases below. For each case, solve as far as possible for $\rho(z)$, $w_A(z)$, $v(z)$, and $T(z)$.

Case A. This is a general case in which the diffusivity and the thermal conductivity are arbitrary functions of composition and temperature

$$D=D(w_A,T) \qquad \text{and} \qquad k_c=k_c(w_A,T)$$

Case B. This is a specific case where the diffusivity is a function of temperature, but not composition, and the thermal conductivity is constant.

$$D=D(T)=D_o\exp\left(-\frac{E_a}{RT}\right) \qquad \text{and} \qquad k_c=k_c$$

where D_o, E_a, and R are constants.

Case C. This is a specific case where both the diffusivity and the thermal conductivity are constant.

$$D=D \qquad \text{and} \qquad k_c=k_c$$

Show all work involved in each step of the derivation. State any additional assumptions that you make.

You may find the following integral useful.

$$\int_{x_{low}}^{x_{high}} \exp\left(\frac{a}{x}\right) dx = x_{high} \exp\left(\frac{a}{x_{high}}\right) - x_{low} \exp\left(\frac{a}{x_{low}}\right) + a\left[Ei\left(1, -\frac{a}{x_{high}}\right) - Ei\left(1, -\frac{a}{x_{low}}\right)\right]$$

where the well-known exponential integral is defined as

$$Ei(n, x) \equiv \int_{1}^{\infty} \frac{\exp(-xt)}{t^n} dt \ .$$

(It is perfectly acceptable to write a solution in terms of Ei.)