Final Exam
ChE 548
Spring, 2006

Problem 1. Molecular Dynamics Simulation

Answer the following questions in terms of (i) the average particle velocity, (ii) the collision diameter, and (iii) the mean free path.

1.A. The Einstein relation for the self-diffusivity applies in the infinite time limit. At short times, a different kind of behavior is observed.

1.A.i. All other things being equal, will a simulation of a fluid at a high density or a low density approach the long-time behavior faster?

1.A.ii. All other things being equal, will a simulation of a fluid at a high temperature or low temperature approach the long-time behavior faster?

1.A.iii. All other things being equal, will a simulation of a fluid at a high molecular weight or a low molecular weight approach the long-time behavior faster?

1.B. Simulations have to undergo a period of "equilibration" during which time they forget their initial configurations (both position and velocities). After the system is equilibrated, then data production can begin. Answer the following questions.

1.B.i. Which will take longer: equilibration of the system or reaching the Einstein long-time limit? Why?

Problem 2. Macroscopic Material, Momentum and Energy Balances

Consider an inviscid, ideal gas flowing down a pipe with circular cross section. Consider only axial variation in properties. The pipe is insulated and there is no heat loss. The inlet conditions are

$$\rho(z=0)=\rho_{in} \tag{1}$$

$$v(z=0)=v_{in} \tag{2}$$

$$T(z=0)=T_{in} \tag{3}$$

The outlet condition is

$$\left.\frac{dT}{dz}\right|_{z=L}=T'_{out} \tag{4}$$

The general material, momentum, and energy balances are

$$\frac{\partial\rho}{\partial t}=-\nabla\cdot(\rho\mathbf{v}) \quad , \tag{5}$$

$$\rho\frac{\partial\mathbf{v}}{\partial t}=-\rho\mathbf{v}\cdot\nabla(\mathbf{v})-\nabla p-\nabla\cdot\boldsymbol{\tau}-\rho\nabla\hat{\Phi} \quad , \tag{6}$$

$$\frac{\partial\rho\left(\frac{1}{2}v^2+\hat{H}+\hat{\Phi}\right)}{\partial t}-\frac{\partial p}{\partial t}=-\nabla\cdot\rho\left(\frac{1}{2}v^2\cdot\mathbf{v}+\hat{H}\mathbf{v}+\hat{\Phi}\mathbf{v}\right)-\nabla\cdot\mathbf{q}-\nabla\cdot(\boldsymbol{\tau}\cdot\mathbf{v}) \quad , \tag{7}$$

2.A. Derive the simplest form of the equations for the steady state profile. State all assumptions made along the way.
2.B. Provide the analytical solution in the limiting case of a negligible thermal conductivity.