Advanced Transport Phenomena II
ChE 548
Department of Chemical Engineering
University of Tennessee, Knoxville
Spring, 2002

Midterm Examination
Administered: March 1, 2002

Problem 1.

For a gas at low density, we can use the mean free path arguments of kinetic theory to obtain an estimate of the self-diffusivity,

$$D_{self,A} = \frac{2}{3}\sqrt{\frac{kT}{\pi m_A}}\frac{1}{\pi \sigma_A{}^2}\frac{1}{n} \qquad \text{(BSL 17.3-9)}$$

In problem 2 of homework 2, you used MD simulations to examine the temperature and density dependence of the self-diffusivity of a low density gas. (See the Table below and attached plots of your work.)

$k = 1.38066 \times 10^{-23}$ J/K/molecule
$N_{av} = 6.02205 \times 10^{23}$ molecules/mole
1 atomic mass unit = 1.66056×10^{-27} kg

Self Diffusion Coefficient for Acetylene at at T = 300K and n = 2.4583×10^{-5} molecules/Å^3	
Team 1	0.73×10^{-5} m^2/s
Team 2	1.33×10^{-5} m^2/s

(a) Consider your self-diffusivity for acetylene (m_A = 26.04 amu, σ_A = 4.114 Å) at T = 300K and n = 2.4583×10^{-5} molecules/Å^3. What is the error between the prediction of kinetic theory and your result? Please report the error as a percent of your simulation result.

(b) Do your simulations confirm or contradict the temperature and density dependence of the self-diffusion coefficient from kinetic theory? Discuss your reasoning.

(c) Using kinetic theory *and* your simulation result for acetylene, please report the self-diffusivity for methane (m_A = 16 amu, σ_A = 3.822 Å) at T = 300K and n = 2.4583×10^{-5} molecules/Å^3.

Problem 2.

You show your microcanonical ensemble MD simulation results to a colleague. He looks at your averge value of the potential energy and the standard deviation of the potential energy (which is equal to the standard deviation of the kinetic energy). He argues that you need to run your simulations for a longer time because your standard deviation of the potential energy is too large relative to the average value. You have already performed a sensitivity analysis on the number of time steps and determined that the average potential energy was not a function of simulation duration. Does your colleague have a legitimate point? If so, why? If not, how do you explain to your colleague that he is wrong?