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,

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

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 \times 10^{-27} \) kg

<table>
<thead>
<tr>
<th>Team</th>
<th>Self Diffusion Coefficient for Acetylene at T = 300K and n = 2.4583 \times 10^{-5} molecules/Å³</th>
</tr>
</thead>
<tbody>
<tr>
<td>Team 1</td>
<td>0.73 \times 10^{-5} m²/s</td>
</tr>
<tr>
<td>Team 2</td>
<td>1.33 \times 10^{-5} m²/s</td>
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</tbody>
</table>

(a) Consider your self-diffusivity for acetylene (\( m_A = 26.04 \) amu, \( \sigma_A = 4.114 \) Å) at T = 300K and n = 2.4583 \times 10^{-5} molecules/Å³. 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, \( \sigma_A = 3.822 \) Å) at T = 300K and n = 2.4583 \times 10^{-5} molecules/Å³.

Problem 2.
You show your microcanonical ensemble MD simulation results to a colleague. He looks at your average 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?