ChE 548  
Assignment III  
Spring 2002

<table>
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<tr>
<th>Team 1.</th>
<th>Team 2.</th>
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Each Team Must Complete the following tasks.

1. Simulate a mixture of methane and ethane in the liquid phase at \( T = 100 \text{ K} \) and approximately 1 atm. Run 4 simulations using methane mole fractions of 0.2, 0.4, 0.6, and 0.8. Use the Lennard-Jones EOS and mixing rules to predict the fluid density at each composition.

   Also
   - Explicitly report pressure, self-diffusivities and potential energy with error bars.
   - Explicitly report all parameters used in the simulation.
   - Use the values of rcut, rmbr, maxeqb, maxstp, N, \( \Delta t \) that you determined to be legitimate from homework set 2, part 1.
   - Determine the thermodynamic correction factor to be used in the Darken equation, using (i) the ideal gas law, (ii) the van der Waals equation of state, and (iii) the Peng-Robinson equation of state.
   - Provide a plot of (i) the self-diffusivities, (ii) the pressure, (iii) the potential energy, (iv) the thermodynamic correction factor (for all 3 EOS), and (v) the transport diffusivity (for all 3 EOS) as a function of mole fraction. Include error bars on the first three plots.
   - Be prepared to justify in class the trends observed in all five plots.
   - Predict the transport diffusivity of this system using three methods:
     a) use kinetic theory, eqn 17.3-10
     b) use Chapman-Enskog theory, eqn 17.3-11
     c) use eqn (17.2-3) and figure 17.2-1

   Suggestions
   - I suggest a timestep of 2 fs and a minimum simulation duration of 50,000 production steps. I suggest a system size of at least 500 molecules, because you need at least 100 molecules of each species to get reasonable statistics and at 0.2 mole fraction, you will have only 100 molecules of component 1, if your total number of molecules is 500.

2. Repeat problem one in the gas phase, where \( T = 400 \text{ K} \) and the pressure is approximately 1 atm. Again run 4 simulations using methane mole fractions of 0.2, 0.4, 0.6, and 0.8. Use the Lennard-Jones EOS and mixing rules to predict the fluid density at each composition. Repeat all parts of problem 1. (In other words, this homework requires that you submit 10 plots.)

   Suggestions
   - I suggest a timestep of 5 fs and a minimum simulation duration of 200,000 production steps. I suggest a system size of at least 500 molecules.