

ChE 548
Homework Assignment III
Spring, 2009

Each Team Must Complete the following two tasks.

Task 1. Simulate a binary mixture of methane and ethane in the gas phase at $T = 400$ K and 1 atm at mole fractions of methane of 0.0, 0.5 and 1.0.

First,

- Use the NpT code to predict the fluid densities of each of the three simulations.
- Verify that your simulation is sufficiently long by showing plots of the MSD vs time on both normal and logarithmic axes.
- Explicitly report pressure, density, self-diffusivity of both components and potential energy with error bars.
- Explicitly report all parameters used in the simulation.

Second, prepare an oral presentation summarizing your results in an organized manner.

- This report must contain all the tasks listed above summarized in graphical or tabular (or both) form.
- Compare the (i) magnitude and (ii) composition-dependence of your pressure with the ideal gas law.
- Compare the (i) magnitude and (ii) composition-dependence of your self-diffusivity with the prediction of Kinetic Theory.
- Calculate a Fickian Diffusivity for the 50/50 mixture using the Darken equation and compare with the prediction from BSL based on Kinetic Theory.

Task 2. Simulate a binary mixture of methane and ethane in a denser phase (relative to task one) at $T = 300$ K and approximately 1000 atm at mole fractions of methane of 0.0, 0.5 and 1.0.

First,

- Use the NpT code to predict the fluid densities of each of the three simulations.
- Verify that your simulation is sufficiently long by showing plots of the MSD vs time on both normal and logarithmic axes.
- Explicitly report pressure, self-diffusivity of both components and potential energy with error bars.
- Explicitly report all parameters used in the simulation.

Second, prepare an oral presentation summarizing your results in an organized manner.

- This report must contain all the tasks listed above summarized in graphical or tabular (or both) form.
- Compare the (i) magnitude and (ii) composition-dependence of your pressure with the Lennard-Jones equation of state.
- Compare the (i) magnitude and (ii) composition-dependence of your self-diffusivity with the prediction from the corresponding states chart in Chapter 17 of BSL 2..
- Calculate a Fickian Diffusivity for the 50/50 mixture using the Darken equation and compare with the prediction from BSL based on the corresponding states chart.