CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #2

1. Molecular-Level Description of Reaction Kinetics

(a) What is the transition state of a chemical reaction?
(b) What is the relationship between the energy of the transition state and the activation energy of a reaction?
(c) In the common expression,

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

what are they physical meanings of k_o and $\exp\left(-\frac{E_a}{RT}\right)$?

(d) Where is the entropy difference hidden in this equation?

2. Continuum-Level Description of Reaction Kinetics

Fogler P3-4.

3. Experimental Determination of Reaction Kinetics

Consider the bimolecular reaction

A + B → D

The concentration of A is measured as a function of time in an isothermal batch reactor. The reactor is run independently at five different temperatures. Assume the reaction obeys the Arrhenius expression. Use "data set one" located at

http://utkstair.org/clausius/docs/ftp/projdata01.zip

You will only need the first three columns of data set one that provide respectively the temperature of the reactor, the time and the concentration of A. The initial concentration of A for all runs is 2.0 mol/liter. The initial concentration of B for all runs is 2.5 mol/liter.

(a) Write the rate as a function of the concentrations of A and B.
(b) Integrate the rate expression to obtain a relationship between the concentration of A, the temperature and k_o and E_a.
(c) Linearize the equation and generate an Arrhenius plot.
(d) Perform a linear regression and determine k_o and E_a.