Final Exam
Administered: Monday, December 8, 2014
8:00 AM – 10:00 AM
28 points

Problem 1. (8 points)

Consider the dimerization reaction:

$$2A \rightarrow B$$

The reaction rate is given by

$$rate = C_A^2 k_o e^{-\frac{E_a}{RT}} \qquad \text{[moles/m}^3\text{/sec]}$$

where

concentration of A: C_A [moles/m^3]
prefactor: k_o [m^3/(moles·sec)]
activation energy for reaction: E_a [Joules/mole]
constant: $R = 8.314$ [Joules/mole/K]
temperature: T [K]

Determine the rate constants, k_o and E_a, from experimental data. The reaction is measured at a constant concentration of A, C_A = 2000 mol/m^3, over a range of temperatures. The rate is recorded. The rate as a function of temperature is given in tabular form in the file "xm4p01_f14.txt" on the exam portion of the course website.

Problem 2. (6 points)

The gamma function is defined as

$$\Gamma(\alpha) = \int_0^\infty x^{\alpha-1} e^{-x} dx \quad \text{for } \alpha > 0$$

(a) Evaluate the gamma function for α = 5 using the intrinsic gamma function. You likely will need to use the `format long` statement in MatLab to get enough digits to display.
(b) How many intervals so you need in the second-order Simpson's method to obtain this result to four significant digits? What did you use as your upper limit of integration?

(over)

Problem 3. (8 points)

Consider the dimerization reaction:

$$2A \rightarrow B$$

The reaction rate is given by

$$rate = C_A^2 k_o e^{-\frac{E_a}{RT}} \qquad \text{[moles/m}^3\text{/sec]}$$

where

concentration of A: C_A [moles/m^3]
prefactor: k_o [m^3/(moles·sec)]
activation energy for reaction: E_a [Joules/mole]
constant: $R = 8.314$ [Joules/mole/K]
temperature: T [K]

If this reaction were to take place in a continuous stirred tank reactor, the mole balances on A and B would have the form

$$\text{accumulation} = \text{in} - \text{out} + \text{generation}$$

$$V\frac{dC_A}{dt} = C_{A,in}F - C_A F - 2rate \qquad (1)$$

$$V\frac{dC_B}{dt} = C_{B,in}F - C_B F + rate \qquad (2)$$

Equations (1) and (2) represent a set of two non-linear coupled ordinary differential equations.

Assume the following parameter values:

inlet concentration of A: $C_{A,in} = 2{,}000$ [moles/m^3]
inlet concentration of B: $C_{B,in} = 0$ [moles/m^3]
prefactor: $k_o = 0.90$ [m^3/(moles·sec)]
activation energy for reaction: $E_a = 66{,}000$ [Joules/mole]
temperature: $T = 600$ [K]
reactor volume: $V = 1$ [m^3]
flowrate: $F = 0.01$ [m^3/sec]

Also, assume that reactor initially has no A or B in it, so that the initial conditions are given by

initial concentration of A: $C_A(t=0) = 0$ [moles/m^3]
initial concentration of B: $C_B(t=0) = 0$ [moles/m^3]

Numerically solve the ordinary differential equations.
(a) Sketch the plot of the concentrations for A and B.
(b) Report values of the concentrations of A and B at time 200 sec.
(c) Report values of the concentrations of A and B at time 500 sec.
(d) Report values of the concentrations of A and B at time 1000 sec.

Problem 4. (6 points)

Consider the system exactly as given in Problem 3. Now consider the system at steady state, where the accumulation term on the left hand sides of equation (1) and (2) are set to zero, yielding

$$0 = C_{A,in}F - C_A F - 2rate \tag{3}$$

$$0 = C_{B,in}F - C_B F + rate \tag{4}$$

Equations (3) and (4) represent a set of two non-linear algebraic equations.

Numerically solve the ordinary differential equations.
(a) State a reasonable set of initial guesses for the concentrations of A and B.
(b) Report the converged values of the concentrations of A and B.
(c) Compare these results to the results from problem 3.