Final Exam
Administered: Monday, December 10, 2018
10:15 AM – 12:15 PM
24 points

Problem 1. (6 points)

Diffusion in solids is often an activated process, in with the diffusivity can be approximated by an Arrhenius-type temperature dependence.

$$D = D_o \, exp\left(-\frac{E_a}{RT}\right)$$

where D is the diffusivity, T is the temperature, R is the gas constant (8.314 J/mol/K), E_a is the activation energy and D_o is the exponential prefactor.

(a) Linearize this equation so that it is linear in the unknown parameters, E_a and D_o.
(b) Using the table of data providing D and T in the file "xm4p01_f18.txt" on the exam portion of the course website, perform a linear regression to determine the mean values of E_a and D_o for this data.
(c) Also report the standard deviations of E_a and D_o.

Problem 2. (6 points)

Consider the following steady-state mass and energy balance for a non-isothermal continuous stirred tank reactor with an irreversible first order reaction:

$$0 = F_{in}C_{A,in} - F_{out}C_A - C_A V k_o e^{-\frac{E_a}{RT}}$$
$$0 = \Delta H_r C_A k_o e^{-\frac{E_a}{RT}} - \dot{Q}$$

where $F_{in} = F_{out} = 10.0\ l/s$, $C_{A,in} = 1.0\ mol/l$, $V = 100.0\ l$, $k_o = 1.0 \cdot 10^{-1}$ 1/s, $E_a =$ 10.0 kJ/mol, $\Delta H_r = 50.0\ kJ/mol$, $\dot{Q} = 0.2\ kJ/l/s$ and $R = 0.008314\ kJ/mol/K$.

(a) Is this system of equations linear or nonlinear?
(b) What is the appropriate technique to solve this system of equations?
(c) Determine the steady values of the outlet concentration of A, C_A, and the temperature, T.

Problem 3. (8 points)

Consider the following transient mass and energy balance for a non-isothermal continuous stirred tank reactor with an irreversible first order reaction:

$$V\frac{dC_A}{dt} = F_{in}C_{A,in} - F_{out}C_A - C_A V k_o e^{-\frac{E_a}{RT}}$$

$$C_p\frac{dT}{dt} = \Delta H_r C_A k_o e^{-\frac{E_a}{RT}} - \dot{Q}$$

where all the variables are the same as they were in problem 2 and the heat capacity per unit volume, $C_p = 2.3\ kJ/l/K$.

(a) Is this system of ordinary differential equations linear or nonlinear?
(b) What is the appropriate technique to solve this system of equations?
(c) Solve the transient behavior of the concentration of A, C_A, and the temperature, T, up to 1000 seconds, if the initial concentration of the reactor is $C_{A,o} = C_{A,in}$ and the initial temperature is $T_o = 400.0\ K$. Sketch a plot of the concentration and temperature.
(d) Report values of the concentration of A, C_A, and the temperature, T at 1000 seconds.

Problem 4. (4 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 $\alpha = 6$ using the intrinsic gamma function in Matlab, `gamma`. 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?