Final Exam
Administered: Friday, December 4, 2020
10:30 AM – 12:45 PM
20 points

Problem 1. (8 points)

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

$$\frac{dC_A}{dt} = \frac{F_{in}}{V} C_{A,in} - \frac{F_{out}}{V} C_A - r_{rxn}$$
$$\frac{dT}{dt} = \frac{\Delta H_r}{C_p} r_{rxn} - \frac{\dot{Q}}{C_p}$$

where the reaction rate is given by $r_{rxn} = C_A^2 k_o e^{-\frac{E_a}{RT}}$

and where $F_{in} = F_{out} = 12.0\ l/s$, $C_{A,in} = 3.0\ mol/l$, $V = 100.0\ l$, $k_o = 0.8 \cdot 10^{-1}$ 1/s, $E_a =$ 10.0 kJ/mol, $\Delta \dot{H}_r = 52.0\ kJ/mol$,$\dot{Q} = 0.2\ kJ/l/s$, $R = 0.008314\ kJ/mol/K$, and $C_p = 2.6\ kJ/l/K$.

(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 500 seconds, if the initial concentration of the reactor is $C_{A,o} = C_{A,in}$ and the initial temperature is $T_o = 350.0\ K$. Sketch a plot of the concentration and temperature.
(d) Report values of the concentration of A, C_A, and the temperature, T at 500 seconds.

Problem 2. (8 points)

The Hall-Petch equation states that the yield strength, σ_y, varies with grain size, d, according to

$$\sigma_y = \sigma_o + k_y \frac{1}{\sqrt{d}} \qquad (1)$$

where σ_o and k_y are material-specific parameters.
[Materials Science and Engineering: An Introduction, 5th Edition, William D. Callister, John Wiley & Sons, Inc., New York, 2000, p. 167.]

For the σ_y vs d data given in the file, http://utkstair.org/clausius/docs/mse301/data/xm4p02_f20.txt, perform the following tasks. The grain size is given in mm and the yield strength in MPa.

(a) Identify all variables, $y = mx + b$, when equation (1) is linearized.
(b) Report the best value of σ_o and k_y.
(c) Report the standard deviations of σ_o and k_y.
(d) Report the measure of fit.

(over)

Problem 3. (4 points)
It has been observed that the relative weight gain, W, as a function of time, t, due to formation of oxides on metals follows the following functional form [Materials Science and Engineering: An Introduction, 5th Edition, William D. Callister, John Wiley & Sons, Inc., New York, 2000, p. 593.]

$$W(t) = K_1 \, ln(K_2 t + K_3)$$

where three empirically determined constants appear and time is measure in days. This expression arises from a weight gain rate equation of the form

$$\frac{dW(t)}{dt} = \frac{K_1 K_2}{K_2 t + K_3}$$

For a surface with a composition gradient, the constants become dependent on the local composition and are therefore functions of time. We propose a form

$$K_1(t) = c_1 \exp\left(-\frac{(t - t_{\max})^2}{s_1}\right)$$

such that the weight gain is now given by

$$W(t) = \int_{t=0}^{t} \frac{K_1(t) K_2}{K_2 t + K_3} dt$$

(a) What method could be used to evaluate the weight gain as a function of time?
(b) Determine the weight gain of such a model at t = 12 days with the following parameters: $c_1 = 0.4$, $s_1 = 7.0$, $t_{max} = 5.0$, $K_2 = 9.0$, and $K_3 = 8.0$.