Final Examination
May 2, 2017

Problem 1. (50%)
Consider a continuous stirred-tank reactor operated under isothermal conditions in which the following three reactions take place:

$$A+B\xrightarrow{k_1}C \qquad A+C\xrightarrow{k_2}D \qquad B+C\xrightarrow{k_3}E \tag{1}$$

The rates of the three irreversible reactions are given by an elementary mechanism,

$$r_1=k_1[A][B] \qquad r_2=k_2[A][C] \qquad r_3=k_3[B][C] \tag{2}$$

The material balances for the reactor are given by (accumulation = in – out +/- generation/consumption):

$$\frac{d[A]}{dt}=F[A]_{in}-F[A]-r_1-r_2 \tag{3.A}$$

$$\frac{d[B]}{dt}=F[B]_{in}-F[B]-r_1-r_3 \tag{3.B}$$

$$\frac{d[C]}{dt}=F[C]_{in}-F[C]+r_1-r_2-r_3 \tag{3.C}$$

$$\frac{d[D]}{dt}=F[D]_{in}-F[D]+r_2 \tag{3.D}$$

$$\frac{d[E]}{dt}=F[E]_{in}-F[E]+r_3 \tag{3.E}$$

Consider a specific case where the volumetric flowrate per unit volume F = 0.1 1/s and the inlet concentrations $[A]_{in}=[B]_{in}=1.0$ mol/liter & $[C]_{in}=[D]_{in}=[E]_{in}=0.0$ mol/liter. Assume the reactor is initially empty, $[A]=[B]=[C]=[D]=[E]=0.0$ mol/liter at t = 0.

An experiment is performed in which the concentrations of the five species are measured as a function of time. This data is recorded in the file located at http://www.utkstair.org/clausius/docs/mse510/data/mse510_xm02_p01_s17.txt . The data file contains six columns corresponding to time, and the concentrations of A, B, C, D and E.

Using this information, determine the optimal values of the three reaction rate constants, k_1, k_2 and k_3. The magnitude of these rate constants should all be on the order of one. Also report the value of the objective function.

Problem 2. (50%)

The one-dimensional heat equation can describe heat transfer in a rutile TiO_2 with both heat conduction and radiative heat loss.

$$\frac{\partial T}{\partial \mathrm{t}} = \frac{k}{\rho C_p} \frac{d^2 T}{dz^2} - \frac{\varepsilon \sigma S}{\rho C_p} \left(T^4 - T_s^{\ 4} \right)$$

where the following variables [with units] are given as

temperature in the material T [K]
surrounding temperature $T_s = 800$ [K]
axial position along material z [m]
thermal conductivity $k = 9.0$ [J/K/m/s]
mass density $\rho =$ 4250 [kg/m^3]
heat capacity $C_p = 711.3$ [J/kg/K]
Stefan–Boltzmann constant $\sigma = 5.670373x10^{-8}$ [J/s/m^2/K^4]
gray body permittivity $\varepsilon = 0.79$
surface area to volume ratio $S = 200$ [m^{-1}] (for a cylindrical rod of diameter 0.05 m)

A rutile TiO_2 cylindrical rod of diameter 0.05 m and length 0.4 m is initially at $T(z, t = 0) = 1000$ K. One end of the rod is maintained at $T(z = 0, t) = 1000$ K. The other end of the rod is maintained at $T(z = L, t) = 1500$ K.

(a) Sketch the transient behavior.
(b) Find the approximate steady-state temperature in the material at z=0.2 m.