ChE/MSE 505
Advanced Engineering Mathematics
Fall 2008

Homework 2

Problem 1. Consider an adiabatic continuously-stirred tank reactor (CSTR) in which the following isomerization reaction takes place

$$A \rightarrow B \tag{1}$$

The rate of this elementary reaction is given by

$$rate = kC_A \tag{2}$$

where C_A is the concentration of A in the tank (and tank effluent) and the rate constant, k, is defined as

$$k = k_o \exp\left(-\frac{E_a}{RT}\right) \tag{3}$$

where the rate prefactor, k_o = 4.48x10^6 1/sec, the activation energy, 6.28 x10^4 J/mol, are known. The gas constant is R = 8.314 J/mol/K and T is the temperature in K. The reaction is exothermic, with a heat of reaction ΔH_R = -3.09x10^5 J/mol. The reactant enters the reactor at a rate, Q = 60.0x10^{-3} mol/sec, and an inlet concentration, C_{in} = 3.0 mol/liter and inlet temperature, T_{in} = 298 K. The tank has a constant volume, V = 18 l. The fluid has a density, ρ = 1.0 kg/l and heat capacity, C_p = 4.19x10^3 J/kg/K.

A material balance on component A yields

$$\frac{dC_A(t)}{dt} = \frac{Q}{V}C_{in} - \frac{Q}{V}C_A(t) - kC_A(t) \tag{4}$$

An energy balance on the system yields

$$\frac{dT(t)}{dt} = \frac{Q}{V}T_{in} - \frac{Q}{V}T(t) - \frac{\Delta H_R}{C_p \rho}kC_A(t) \tag{5}$$

Typically, one eliminates the concentration in terms of an extent of reaction, χ, defined as

$$\chi = 1 - \frac{C_A(t)}{C_{in}} \tag{6}$$

where the extent of reaction is bound between 0 (no reaction) and 1 (all reactant consumed). Differentiating equation (6) and substituting in equation (4) yields a new (but equivalent) version of the mass balance in terms of the scaled variable (extent of reaction)

$$\frac{d\chi(t)}{dt} = -\frac{1}{C_{in}}\frac{dC_A(t)}{dt} = -\frac{Q}{V} + \frac{Q}{VC_{in}}C_A(t) + \frac{k}{C_{in}}C_A(t) \qquad (7)$$

Taken together, equations (5) and (7) provide a complete description of the behavior of this reactor.

(a) This reactor has three steady states. Find them. Indicate what method and what initial guess was used to find each of the three steady states. Assign a physical description of each steady state.

(b) Provide a plot of $\chi(t)$ and $T(t)$ versus time for the following three sets of initial conditions.

Set 1: $C_A(t=0) = 3.0$ mol/l and $T(t=0) = 298$ K

Set 2: $C_A(t=0) = 3.0$ mol/l and $T(t=0) = 398$ K

Set 3: $C_A(t=0) = 0.0$ mol/l and $T(t=0) = 398$ K

If you solve the equations in terms of the extent of reaction, you will need to convert the initial concentration into an initial extent of reaction via equation 6.

(c) Compare the long-time solutions of part (b) with your steady state solutions of part (a).

(d) For any of the initial conditions in part (b), does the reactor ever get temporarily hotter than its final steady state? Explain.

Problem 2. Consider the following one-dimensional linear parabolic P.D.E., commonly known as the heat equation:

$$\frac{\partial T}{\partial \mathrm{t}} = \alpha\left(\frac{\partial^2 T}{\partial x^2}\right) + \frac{f(t,x)}{\rho \hat{C}_p} \tag{1}$$

where , α , the thermal diffusivity is defined as

$$\alpha = \frac{k}{\rho C_p} \tag{2}$$

where k is the thermal conductivity, ρ is the density and C_p is the heat capacity. The heat generation term, f, is given by radial heat loss of an uninsulated rod to the surroundings

$$f(x,t) = \frac{h\mathrm{A}\left(\mathrm{T}_{\mathrm{surround}} - T(x,t)\right)}{V} \tag{3}$$

where A is the radial surface area of the rod, V is the volume of the rod, h is the heat transfer coefficient, and $T_{surround}$ is the temperature of the surroundings.

(A) Consider an aluminum cylindrical rod 1.0 meter long connecting two heat reservoirs. One of the reservoirs is maintained at T=300K, the other reservoir at T=400 K. Initially, the cylinder is at 300 K. There is no heat loss from the rod (h=0). Consider the system to be one-dimensional.

(a) Write the IC and BC's.
(b) What does the initial profile look like?
(c) What does the steady state profile look like? Explain.
(d) What is the temperature 0.5 meters into the rod at steady state?
(e) What is the temperature 0.5 meters into the rod after 1000 seconds?
(f) Approximately how long does it take for the midpoint of the rod to get within 1% of the steady state value?
(g) Approximately how long does it take for the midpoint of a lead (Pb) rod to get within 1% of the steady state value? Explain the difference.

(B) Consider an aluminum cylindrical rod 1.0 meter long connecting two heat reservoirs. One of the reservoirs is maintained at T=300K, the other reservoir at T=400 K. Initially, the cylinder is at 300 K. The rod is not insulated so heat is lost from the rod, which has a radius of 5.0 cm. The surrounding temperature is 200 K. Use a heat transfer coefficient of 40.0 W/m^2/K. Consider the system to be one-dimensional.

(a) Write the IC and BC's.
(b) What does the steady state profile look like? Explain.
(c) What is the temperature 0.5 meters into the rod at steady state?
(d) What is the temperature 0.5 meters into the rod after 1000 seconds?
(e) Approximately how long does it take for the midpoint of the rod to get within 1% of the steady state value?
(f) Approximately how long does it take for the midpoint of a copper (Cu) rod to get within 1% of the steady state value? Explain the difference.