Homework Assignment Number Six

Problem (1) Combined diffusion with exothermic reaction problem (transient analysis)

Consider a cylindrical rod of nanoporous solid material. Inside this rod a reactant A is being converted to product B in a first order, irreversible reaction.

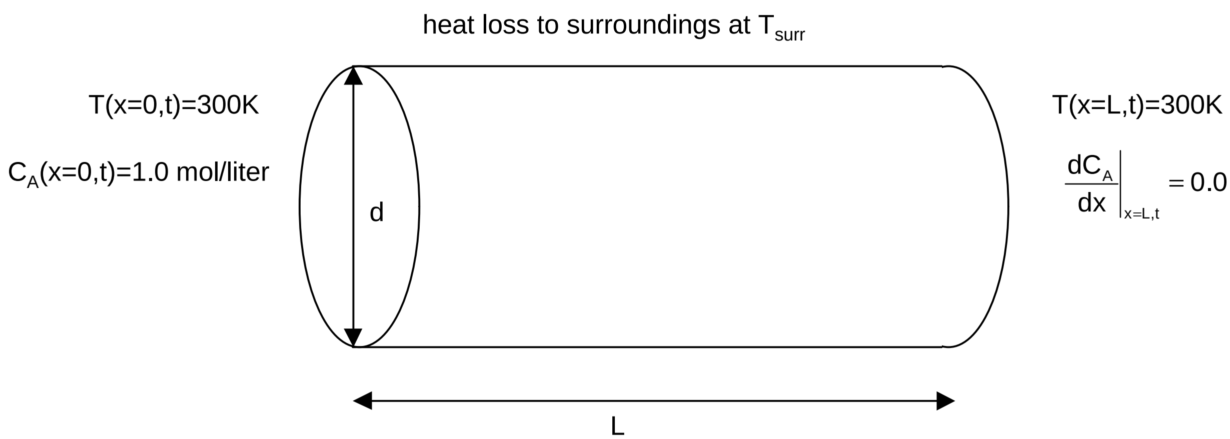

Figure One. Schematic of System

L is the length of the rod and d is the diameter.

If we assume that the distribution of A is uniform in the radial dimension, then a molar balance on component A yields:

acc = in - out + gen

$$\frac{\partial C_A}{\partial t} = D\frac{\partial^2 C_A}{\partial x^2} - kC_A \quad (1)$$

where

- C_A is the concentration of A [moles/liter]
- D is the diffusivity of A in the rod [m^2/sec]
- t is time [sec]
- x is spatial position [m]

The rate constant, k, is given by

$$k = k_o e^{\frac{-E_a}{RT}} \quad (2)$$

where

- k_o is the exponential prefactor [1/sec]
- E_a is the activation energy [Joules/mole]
- T is the temperature [K]
- R is the gas constant [8.314 J/mole/K]

Heat is lost to the surroundings at the surface of the cylinder. Heat is also generated via the exothermic reaction. Therefore an energy balance can be written as

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} - \frac{\Delta H_r k C_A}{\rho C_p} + \frac{h A_{surf}}{\rho C_p V}(T_{surr} - T) \tag{3}$$

where

$$\alpha = \frac{k_c}{\rho C_p}$$

and where

α is the thermal diffusivity [m^2/sec]
ΔH_r is the heat of reaction [J/mol]
ρ is the fluid molar density [mol/liter]
C_p is the fluid heat capacity [J/mol/K]
k_c is the thermal conductivity of the medium[J/m/K/sec]
h is the heat transfer coefficient [J/m^2/K/sec]
A_{surf} is the surface area of the rod [m^2]
V is the volume of the system [m^3]
T_{surr} is the temperature of the surroundings [K]

Initially, the entire nanoporous material contains A at a concentration of $C_{A,o}$ and at a temperature of T_o.

$$C_A(x, t = 0) = C_{A,o} \tag{4.a}$$

$$T(x, t = 0) = T_o \tag{4.b}$$

The temperature and the concentrations at x=0 are maintained at constant values.

$$C_A(x = 0, t) = C_{A,1} \tag{5.a}$$

$$T(x = 0, t) = T_1 \tag{5.b}$$

At the other end of the rod, the flux of A is zero and the temperature is maintained at a constant value.

$$\left.\frac{dC_A}{dx}\right|_{c=L,t} = 0.0 \tag{5.c}$$

$$T(x = L, t) = T_2 \tag{5.d}$$

Thus we have a fully specified system of coupled nonlinear parabolic partial differential equations in one spatial dimension.

Your task is to find the steady state and transient behavior of the Temperature and Concentration of A. You are to submit:

(a) your input file, containing the PDEs. (Not the entire syspde_para.m code.)

(b) The reduced temperature and concentration profiles (T/T_o & $C_A/C_{A,o}$) at time = 10, 100, 1000, 4000, & 16000 seconds. (5 plots total.)

(c) Discussion, including qualitative explanation of the behavior. Which term (diffusion, reaction, or heat loss) dominates in the energy balance? Why? Which term (diffusion or reaction) dominates in the mass balance? Why? Which term is causing the behavior seen in the profiles at time = 100 sec? Why? Which term is causing the behavior seen in the profiles at time = 16000 sec? Why?

parameters:

$C_{A,o} = 1.0$	[moles/liter]
$C_{A,1} = 1.0$	[moles/liter]
$T_o = 400$	[K]
$T_1 = 400$	[K]
$T_2 = 400$	[K]
$D = 1.0 \cdot 10^{-7}$	[m^2/sec]
$L = 0.2$	[m]
$d = 0.01$	[m]
$k_o = 5000.0$	[1/sec]
$E_a = 4 \cdot 10^4$	[Joules/mole]
$R = 8.314$	[J/mole/K]
$\Delta H_r = -5 \cdot 10^6$	[J/mol]
$\rho = 100.0$	[kg/m^3]
$C_p = 4000.0$	[J/kg/K]
$k_c = 200.0$	[J/m/K/sec]
$h = 4.0$	[J/m^2/K/sec]
$A_{surf} = \pi d L$	[m^2]
$V = \pi \frac{d^2}{4} L$	[m^3]
$T_{surr} = 250$	[K]

Problem (2) Solve a single hyperbolic PDE.

$$\frac{\partial^2 U}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 U}{\partial t^2}$$

where $c = 2$.

Use the following initial and boundary conditions.

$$U(x=0,t) = 0.0$$
$$U(x=L,t) = 0.0$$

$$U(x, t = 0) = a\left(x^2 - Lx\right) + b \cdot \sin\left(\frac{6\pi x}{L}\right)$$

$$\frac{dU}{dt}(x, t = 0) = 0.0$$

where L = 2.0 and a = 0.01 and b= 0.001. I was able to solve this problem from time = 0 to 2.5 seconds, using 40 spatial intervals and 1000 temporal intervals.
Turn in a plot of the position and velocity for t = 0, 1, and 2.5 seconds.

Problem (3) Solve a single elliptic PDE.

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = f(x, y) = 0$$

Use the following boundary conditions.

$$U(x = 0, y) = 0.0$$

$$U(x = 1, y) = \frac{y}{20}$$

$$U(x, y = 0) = 0.0$$

$$U(x, y = 1) = \frac{1}{20}\sin\left(\frac{\pi x}{2}\right)$$

Show the U profile.