CE 561 Homework 9: Assigned 11/02/09, due 11/09/09

(1) In class, we derived a set of partial differential equations that, with some assumptions, govern the spatial and temporal behavior of species concentrations in a chemically reacting system.

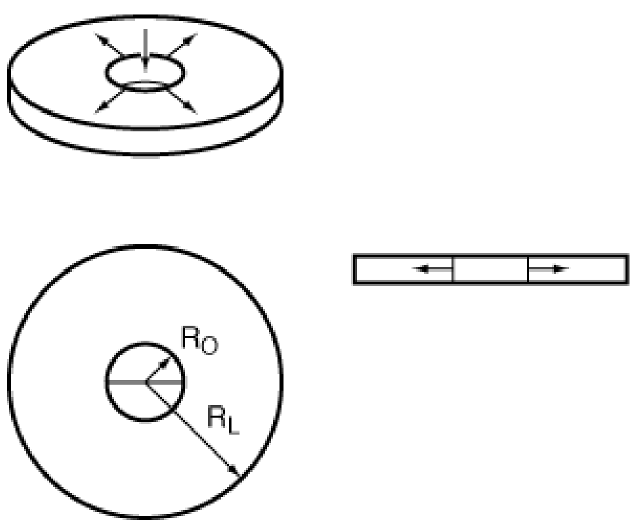
$$\frac{dC_k}{dt} = -\underline{v} \cdot \nabla C_k + D_k \nabla^2 C_k + \sum_{i=1}^{M} \alpha_{ik} r_i \text{, for } k \text{ from 1 to } N\text{, the number of species.}$$

If the reactor to be modeled has turbulent flow or has complex flow patterns through a bed of catalyst, then the diffusion coefficients, D_k are not molecular diffusion coefficients. Instead, they are effective diffusion coefficients that are related to mixing in turbulent eddies and in complex flow patterns past catalyst particles. In that case, the diffusion coefficients are the same for all of the species. We can define extents of reaction such that the species concentrations are related to the extents of reaction by

$$C_k = C_{k,o} + \sum_{i=1}^{M} \alpha_{ik} \xi_i$$

where the $C_{k,o}$ are some reference concentrations (usually the feed concentrations) and the ξ_i are the extents of reaction (with units of concentration). Starting from the above PDE's for the concentrations (with the same effective diffusion coefficient for all species) and this definition of the extents of reaction, derive a set of M equations in terms of the extents of reaction that are equivalent to the N equations in terms of the concentrations.

(2) Radial-flow reactors, like the one shown schematically here, can be used to good advantage for exothermic reactions with high heats of reaction.



The high radial velocities at the entrance to the reactor are useful in reducing hot spots within the reactor. As fluid moves through the reactor, the fluid velocity decreases, so that the highest velocity is near the entrance of the reactor where the reactant concentration is highest and the heat release is greatest. The reactants flow into the reactor at radius R_o and flow out of the reactor at radius R_L. The thickness of the reactor is h. Heat flows out of the reactor through the top and bottom surfaces to a cooling fluid at temperature T_c, and the heat flux (energy per area per time) at these surfaces can be written as $q = U(T - T_c)$. In this problem, you will derive appropriate governing equations to describe the concentrations and temperature in this reactor.

(a) If the density, heat capacity, thermal conductivity, and diffusion coefficients are constant, we can start from the 'general' equations derived in class.

$$\frac{dC_k}{dt} = -\underline{v} \cdot \nabla C_k + D_k \nabla^2 C_k + \sum_{i=1}^{M} \alpha_{ik} r_i \quad \text{(for } k \text{ from 1 to } N\text{)}$$

$$\rho \hat{C}_p \frac{dT}{dt} = -\rho \hat{C}_p \underline{v} \cdot \nabla T + \lambda \nabla^2 T + \sum_{i=1}^{M} (-\Delta H_i) r_i + \sum_{k=1}^{N} \left(C_{pk} \left(T - T_{ref} \right) D_k \nabla^2 C_k + C_{pk} D_k \nabla T \cdot \nabla C_k \right)$$

Apply these equations to the radial flow reactor geometry by writing them in terms of a radial coordinate r and axial (thickness) coordinate z. Specify appropriate boundary conditions for the concentrations and temperature at the inlet ($r = R_o$), outlet ($r = R_L$), top ($z = h/2$) and bottom ($z = -h/2$). Note that the velocity will vary with position, since it must be zero at the upper and lower surfaces. You do not need to consider the momentum balance, though – treat the velocity as known.

(b) Simplify the equations from part (a) by making the approximation that the velocity is zero in the axial direction. Then the velocity only has a radial component, and this component depends on r but does not depend on z. You can find this velocity in terms of the inlet velocity (or flow rate) using the overall mass balance.

(c) Further simplify the equation from part (b) by assuming that the temperature and concentrations are also uniform in the axial direction. The equations will now become one-dimensional (there will only be variations in the radial direction). Be careful to treat the heat flow through the top and bottom surfaces correctly when you convert this from a 2-D to a 1-D problem.

(d) Further simplify the result from part (c) by assuming that dispersion (diffusion) in the radial direction is negligible compared to convection and reaction.

(e) Instead of starting from the general equation to get to the result obtained in part (c), start by assuming that the concentrations, temperature, and velocity are uniform across the thickness of the reactor. Then derive governing equations for the situation by making mass, energy, and species balances on an annular control volume of axial thickness h (the whole thickness of the reactor) and radial dimension dr (volume from r to $r + dr$). You should arrive at the same results as in part (c).

(3) Our favorite reaction, A ↔ B with reaction rate $r = k_1C_A - k_2C_B$ is to be carried out in an ideal batch reactor. The reactor temperature is constrained to lie between 550 K and 750 K. The feed concentrations are C_{Ao} = 1.1 kgmol/m^3, and C_{Bo} = 0.2 kgmol/m^3. The desired outlet composition is C_A = 0.6 kgmol/m^3 and C_B = 0.7 kgmol/m^3. What is the optimal temperature profile (temperature as a function of batch time to reach the desired outlet composition) for each of the three cases below? What is the batch time required in each case if the optimal temperature profile is followed? Prepare plots of the temperature and concentrations vs. batch time for each case, following the optimal temperature profile.

(a) $k_1 = 1.8\times10^5 \exp(-12000/T)$ min^{-1}, $k_2 = 0$

(b) $k_1 = 1.8\times10^6 \exp(-12000/T)$ min^{-1}, $k_2 = 1.2\times10^{14} \exp(-24000/T)$ min^{-1}

(c) $k_1 = 2.4\times10^{13} \exp(-24000/T)$ min^{-1}, $k_2 = 1.8\times10^4 \exp(-12000/T)$ min^{-1}