CHEG 321: Process Kinetics Due: Friday, November 30th, 2007

Homework #8: Steady-State Operation of Non-Isothermal Reactors

A CSTR is to be designed for carrying out the liquid-phase reaction A → B, which is highly exothermic (ΔH_{rxn} = 350 kJ/mol) and has a large activation energy (E_A = 52 kJ/mol.K), and is carried out in a highly reactive solvent (concentrated hydrogen peroxide, ρ = 1300 g/L; C_p = 0.85 J/gm.K). For these reasons, the reaction is carried out in a small reactor system (V = 2 cm^3) with a cooling system (U = 150 $W/m^2.K$; a = 100 cm^2 ; T_C = 253 K) to maintain safe operating temperatures. The feed is supplied at a "safe" temperature of T_0 = 273 K, and a reactant concentration of 1 mol/L. It is your job to determine whether these are safe operating conditions, by the following analysis:

1. SHOW that the dimensional mass and energy balances may be rendered dimensionless, to obtain the system of equations:

[1'] $$\frac{dx}{d\tau} = 1 - x - Da \cdot x \cdot \exp\left[\gamma\left(1 - \frac{1}{y}\right)\right]$$

[2'] $$\frac{dy}{d\tau} = 1 - y + Da \cdot \beta \cdot x \cdot \exp\left[\gamma\left(1 - \frac{1}{y}\right)\right]$$

By using the definitions:

$$\tau = \frac{t}{\theta},\ x = \frac{A}{A_0},\ y = \frac{T}{T_m},\ \text{where}\ T_m = \left(\frac{T_0 + \delta \cdot T_C}{1+\delta}\right),\ \text{and}\ \delta = \left(\frac{U \cdot a}{\rho \cdot C_p \cdot q}\right).$$

2. What are the definitions of Da, β for the proposed reactor design? SHOW that these are dimensionless values.

3. Using equations [1'] and [2'], show that the dimensionless concentration (x) can be written in terms of (y) as follows:

$$x = 1 + \frac{y-1}{\beta}.$$

4. If 100% conversion is obtained, what is the corresponding maximum temperature achievable in this system?

5. Using the relationship derived in Question (3), show that the energy balance for this system can be re-written as:

$$\frac{1}{Da} = F(y) = \frac{(1+\beta-y)}{y-1} \cdot \exp\left[\gamma\left(1-\frac{1}{y}\right)\right]$$

6. Plot F(y) vs. 1/Da, and use this plot to identify whether multiplicity will occur within this reactor.

7. Using the criteria that $\frac{d}{dy}F(y) < 0$ for global stability, derive the range of flowrates (q) that will result in multiple steady-states, assuming that you cannot change inlet concentrations or temperatures.

8. If the liquid solution decomposes violently at temperatures in excess of 40^{o}C, what is the maximum safe operating conversion and temperature for this reactor? What is/are the corresponding Damkohler # and flow rate(s) to achieve this “safe” conversion?

9. Using the criteria developed in class for global stability (below), and given a fixed inlet concentration (dictated by downstream chemicals), how cold must the coolant temperature be to ensure global stability of this reactor? What damkohler number is then required to achieve 95% conversion? What is the corresponding reactor temperature?

$$\gamma \leq \frac{4 \cdot (1+\beta)}{\beta}.$$

10. Using the criteria developed in class for global stability (above), and given a fixed coolant temperature of 253 K, what is the maximum inlet concentration possible before we lose global stability? What damkohler number is required to achieve 95% conversion? What is the corresponding reactor temperature?