Continuously Stirred Tank Reactor

Development of the Model

Let $C(T)$ be the concentration of the primary reactant in moles per m^3, where T is time, so that the total amount of reactant in volume V is $VC(T)$ moles. Let $U(T)$ be the temperature in K. Then the heat energy in the reactor is $\rho c_p VU$, where ρ is the density in kg/m^3 and c_p is the heat capacity in J/(kg K). Changes in the total amount of reactant and the total amount of heat energy are determined by several physical processes:

1. Fluid flows into the reactor with flow rate q in m^3/sec. This fluid has concentration C_0 and temperature U_0.
2. The well-stirred mixture flows out of the reactor with the same flow rate q.
3. The reactor is cooled at a rate proportional to the difference between the reactor temperature and the inlet temperature U_0, with rate constant h in J/(K sec).
4. The reactant amount decreases at a rate proportional to the amount of reactant, with temperature-dependent rate constant k in sec^{-1}. This rate constant is determined by the Arrhenius formula $k = k_0 e^{-E/RU}$, where E is the activation energy in J/mole and R is the universal gas constant in J/(mole K).
5. The chemical reaction also increases the energy at a rate proportional to the rate of the reaction, with proportionality constant Q in J/mole.

Using these assumptions, we obtain the model

$$V\frac{dC}{dT} = q(C_0 - C) - kVC, \tag{1}$$

$$\rho c_p V\frac{dU}{dT} = \rho c_p q(U_0 - U) - h(U - U_0) + QkVC, \tag{2}$$

$$k = k_0 e^{-E/RU}. \tag{3}$$

Nondimensionalization

The model (1-3) has 11 parameters, along with the constant R. Its analysis is considerably simplified by nondimensionalization, which eliminates some parameters and groups the rest into a small number of dimensionless combinations. To nondimensionalize the model (1-3), we replace the original dimensional variables with dimensionless counterparts using the substitutions

$$T = \frac{V}{q}t, \qquad C = C_0(1 - x), \qquad U = U_0 + \frac{U_0}{\alpha}u. \tag{4}$$

Note that x is the fraction of initial reactant concentration that has been reacted at time t; hence it measures the progress of the reaction, with $x = 0$ for no reaction and $x = 1$ for complete reaction. [The model is slightly easier to analyze using the progress variable x rather than the dimensionless concentration $c = C/C_0$.] The reduced temperature u is set so that $u = 0$ when $U = U_0$ and $u = \alpha$ when $U = 2U_0$. (Keep in mind that U and U_0 are absolute temperatures, so room temperature of 70°F= 21°C would be $U_0 = 294$K; hence, $2U_0 = 588$K= 315°C= 600°F.

With the additional simplification that external cooling is unimportant, the dimensionless model is

$$x' = -x + \mathrm{Da}(1-x)e^{\frac{u}{1+u/\alpha}}, \qquad x(0) = 0; \tag{5}$$

$$u' = -u + \beta\, D(1-x)e^{\frac{u}{1+u/\alpha}}, \qquad u(0) = 0, \tag{6}$$

where α is a dimensionless activation energy, β is a dimensionless measure of how much heat is released by the reaction, and D is a measure of the relative importance of the chemical reaction to the flow when the temperature is U_0. The reactor will be more productive for smaller values of D. This parameter is easily adjusted by controlling the flow rate q.

Simplification

1. Define a new function z by the formula

$$z = u - \beta x. \tag{7}$$

   Use this definition and the initial value problems (7) and (8) to obtain an initial value problem for z.

2. Solve the initial value problem from step 1.

3. Use the definition of z from step 1 and the solution for z from step three to obtain a formula for u as a function of x.

4. Substitute the formula for u into (5) to obtain a single initial value problem for the reactant progress variable x. The resulting equation will contain β in one place and β/α in another. For algebraic convenience, define a new parameter $\delta = \beta/\alpha$.

Your final result from this simplification is a single initial value problem with just two parameters. Part 3 will be the study of this problem using qualitative and numerical methods.