CBE 450 Chemical Reactor Fundamentals
Fall, 2011
Project

Consider a jacketed CSTR in which the following irreversible reaction takes places

$$A + B \rightarrow C + D$$

with elementary mechanism such that the rate of the reaction is

$$r = kC_A C_B$$

where the rate constant is given by

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

The activation energy for the reaction is 65000 J/mol. The rate constant prefactor for the reaction is 1.0e+6 liter/mole/s. The heat capacities of A, B, C, and D and the solvent (S) are respectively 80.0, 140.0, 120.0, 120.0 and 75.3 J/mol/K. The heats of formation of A, B, C, and D at a reference temperature of 298.15 K are respectively -15, -10, -50 and -200 kJ/mol. The inlet flowrate is 10 liters/s. The inlet temperature is 300 K. The inlet concentrations of A, B, C, D and S are 5.0, 5.0, 0.0, 0.0 and 45.6 mol/liter respectively. The volume of the reactor is 500 liters.

The reactor is jacketed. The jacket has a volume of 0.5 m^3. The overall heat transfer coefficient from the reactor to the jacket is 1500.0 J/s/m^2/K and the surface area for heat transfer is 1.5 m^2. Water is used as the heat transfer fluid. The heat capacity of the fluid is 4.184 J/gram/K (75.3 J/mole/K) and the concentration is 55.6 mol/liter. The flowrate of the jacket fluid is 10 liters/s. The fluid is at 273.15 K. The initial temperature of the coolant is the same as the inlet temperature.

Task 1. Consider a case where the jacket is not used (set U = 0) and we consider the reactor to be adiabatic.

(a) Use the Newton-Raphson Method to find the three steady-states of the reactor.

(b) Show some sample transient plots of concentration and temperature vs time to indicate the stability of each of the steady states.

(c) Create a phase plot showing the concentration of A vs the reactor temperature. Indicate on the plot the basins of attraction for the various steady states.

Task 2. Now examine the case with a cooling jacket (U = 1500). Repeat the tasks above and explain how the jacket affects the steady states, transient behavior, and features of the phase plot.