REB, The Course
Class 9 Learning Activity Solution

A 150°C solution containing 2 mol L^{-1} of A is being fed to a 500 L CSTR at a rate of 250 L h^{-1}. A jacket surrounding the CSTR contains molten salt at a constant temperature of 180 °C. The contact area between the CSTR contents and the jacket is 2 m^2 and the overall heat transfer coefficient is equal to 500 kcal m^{-2} h^{-1} K^{-1}. Within the reactor reaction (1) occurs at a rate given by equation (2). The pre–exponential factor for the rate coefficient in equation (2) is 1.14 × 10^9 L mol^{-1} h^{-1} and the activation energy is 16.2 kcal mol^{-1}. The reacting solution has a constant density and a constant heat capacity of 1.17 cal ml^{-1} K^{-1}. The heat of reaction is 18.2 kcal mol^{-1} and is independent of temperature. At steady state, what are the outlet temperature and conversion of A?

$$A \rightarrow Z \tag{1}$$

$$r_1 = k_1 C_A^2 \tag{2}$$

Assignment Summary

Reaction

$$A \rightarrow Z \tag{1}$$

Rate Expression

$$r_1 = k_1 C_A^2 \tag{2}$$

Reactor: Steady-state, liquid-phase, non-isothermal CSTR

Given Constants: T_{in} = (150 + 273.15) K, $C_{A,in}$ = 2 mol L^{-1}, V = 500 L, $\dot{V}_{in}$ = 250 L h^{-1}, T_{ex} = (180 +273.15) K, A = 2 m^2, U = 500 kcal m^{-2} h^{-1} K^{-1}, $k_{0,1}$ = 1.14 × 10^9 L mol^{-1} h^{-1}, E_1 = 16.2 kcal mol^{-1}, $\breve{C}_p$ = 1.17 cal ml^{-1} K^{-1}, and ΔH_1 = 18.2 kcal mol^{-1}.

Deliverables: T and f_A

Formulation of the Equations

Reactor Model Equations:

$$0 = \dot{n}_{A,in} - \dot{n}_A - Vr_1 = \epsilon_1 \tag{3}$$

$$0 = -\dot{n}_Z + Vr_1 = \epsilon_2 \tag{4}$$

$$0 = \dot{Q} - \dot{V}_{in}\breve{C}_p\left(T - T_{in}\right) - Vr_1\Delta H_1 = \epsilon_3 \tag{5}$$

Reactor Model Variables: $\dot{n}_A$, $\dot{n}_Z$, and T

Additional Computable Unknowns: $\dot{n}_{A,in}$, r_1, k_1, C_A, $\dot{V}$, $\dot{Q}$

$$\dot{n}_{A,in} = C_{A,in}\dot{V}_{in} \tag{6}$$

$$\dot{V} = \dot{V}_{in} \tag{7}$$

$$k_1 = k_{0,1}\exp\left(\frac{-E_1}{RT}\right) \tag{8}$$

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{9}$$

$$\dot{Q} = UA\left(T_{ex} - T\right) \tag{10}$$

ATE Solver Inputs:

1. Initial guesses for the reactor model variables

$$\dot{n}_{i,guess} = \dot{n}_{i,in} \qquad i = A \text{ and } Z \tag{11}$$

$$T_{guess} = T_{in} - 5K \tag{12}$$

2. Residuals function that
    a. receives guesses for the reactor model variables
    b. returns the residuals corresponding to the reactor model equations

Deliverables Equation:

$$f_A = \frac{\dot{n}_{A,in} - \dot{n}_A}{\dot{n}_{A,in}} \tag{13}$$

Implementation of the Calculations

The Python script, activity_9.py, that was written to perform the calculations accompanies this solution.

Results and Discussion

The calculations were performed as described above. The conversion is 85.6% and the outlet temperature is 167 °C. If the reactor had operated adiabatically, the outlet temperature would have been less than 150 °C (the feed temperature) because the reaction is endothermic. That, in turn would have resulted in a lower conversion. The outlet temperature is greater than the feed temperature because the external fluid gave more heat to the reacting fluid that was consumed by the endothermic reaction..

Deliverables

The temperature of the fluid leaving the steady-state CSTR described in the assignment narrative is 167 °C, and 85.6% of the reagent A fed to it is converted to Z.