REB, The Book
Example 6.6.1 Solution

The amount of A, (10%), in a gas mixture with B (65%), and inert, I, (25%) at 165 °C and 5 atm needs to be reduced to 0.1%. This is going to be accomplished by converting the A into Z according to reaction (1). An adiabatic, steady-state CSTR is going to be used. The rate expression is given in equation (2) where the pre-exponential factor is 1.37 x 10^5 m^3 mol^{-1} min^{-1} and the activation energy is 11,100 cal mol^{-1}. The heat of reaction is constant and equal to –7200 cal mol^{-1}, and the heat capacities of A, B, I, and Z are equal to 7.6, 8.2, 4.3, and 13.8 cal mol^{-1} K^{-1}, respectively. What space time is required, and what temperature will result?

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

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

Assignment Summary

Reaction

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

Rate Expressions

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

Reactor: Adiabatic, steady-state CSTR

Given Constants: $y_{A,in}$ = 0.1, $y_{B,in}$ = 0.65, $y_{I,in}$ 0.25, T_{in} = (165 +273.15) K, P = 5 atm, y_A = 0.001, $k_{0,1}$ = 1.37 x 10^5 m^3 mol^{-1} min^{-1}, E_1 = 11,100 cal mol^{-1}, ΔH_1 = –7200 cal mol^{-1}, $\hat{C}_{p,A}$ = 7.6 cal mol^{-1} K^{-1}, $\hat{C}_{p,B}$ = 8.2 cal mol^{-1} $^{-1}$, $\hat{C}_{p,I}$ = 4.3 cal mol^{-1} K^{-1}, and $\hat{C}_{p,Z}$ = 13.8 cal mol^{-1} K^{-1}.

Basis: $\dot{V}_{in}$ = 1.0 m^3 min^{-1}

Deliverables: τ and T

Formulation of the Equations

Reactor Model Equations:

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

$$0 = \dot{n}_{B,in} - \dot{n}_B - Vr_1 = \epsilon_2 \quad (4)$$

$$0 = \dot{n}_{I,in} - \dot{n}_I = \epsilon_3 \quad (5)$$

$$0 = -\dot{n}_Z + Vr_1 = \epsilon_4 \quad (6)$$

$$0 = -\left(\dot{n}_{A,in}\hat{C}_{p,A} + \dot{n}_{B,in}\hat{C}_{p,B} + \dot{n}_{I,in}\hat{C}_{p,I}\right)\left(T - T_{in}\right) - Vr_1\Delta H_1 = \epsilon_5 \quad (7)$$

Reactor Model Variables: V, $\dot{n}_B$, $\dot{n}_I$, $\dot{n}_Z$, and T

Additional Computable Unknowns: $\dot{n}_{A,in}$, $\dot{n}_A$, r_1, k_1, C_A, C_B, $\dot{n}_{B,in}$, and $\dot{n}_{I,in}$

$$\dot{n}_{A,in} = y_{A,in}\frac{P\dot{V}_{in}}{RT} \quad (8)$$

$$y_A = \frac{\dot{n}_A}{\dot{n}_A + \dot{n}_B + \dot{n}_I + \dot{n}_Z} \quad \Rightarrow \quad \dot{n}_A = \frac{\left(\dot{n}_B + \dot{n}_I + \dot{n}_Z\right)y_A}{1 - y_A} \quad (9)$$

$$r_1 = k_1 C_A C_B \quad (2)$$

$$k_1 = k_{0,1}\exp\left(\frac{-E_1}{RT}\right) \quad (10)$$

$$C_A = \frac{\dot{n}_A}{\dot{n}_A + \dot{n}_B + \dot{n}_I + \dot{n}_Z}\frac{P}{RT} \quad (11)$$

$$C_B = \frac{\dot{n}_B}{\dot{n}_A + \dot{n}_B + \dot{n}_I + \dot{n}_Z}\frac{P}{RT} \quad (12)$$

$$\dot{n}_{B,in} = y_{B,in}\frac{P\dot{V}_{in}}{RT} \tag{13}$$

$$\dot{n}_{I,in} = y_{I,in}\frac{P\dot{V}_{in}}{RT} \tag{14}$$

ATE Solver Inputs:

1. Initial guesses for the reactor model variables.

$$V_{guess} = 1\,m^3 \tag{15}$$

$$\dot{n}_{i,guess} = \dot{n}_{i,in} \qquad i = B, I, \text{ and } Z \tag{16}$$

$$T_{guess} = T_{in} + 5\,K \tag{17}$$

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

Deliverables Equation:

$$\tau = \frac{V}{\dot{V}_{in}} \tag{18}$$

Implementation of the Calculations

The Python script, example_6_6_1.py, that was written to perform the calculations accompanies this solution.

Results and Discussion

The ATE solver converged using the initial guess shown in equations (15) through (17). In this analysis, the initial composition and the conversion were specified. As such, the amount of heat released is fixed, and since the reactor is adiabatic, that also fixes the final temperature. Consequently, there is no need to check for other steady states.

The outlet temperature is 265 °C and the space time required to reach the specified outlet mole fraction of A is 0.42 min. The increase in temperature is expected because the reactor is adiabatic and the reaction is exothermic.

Deliverables

A space time of 0.42 min is required to reduce the amount of A to 0.1%. Doing so will increase the temperature of the gas mixture to 265 °C.