REB, The Course
Class 17 Practice Assignment Solution

Irreversible gas phase reaction (1) is exothermic with a heat of reaction equal to –12.9 kcal mol^{-1}. The rate expression is presented in equation (2), where the pre-exponential factor equals 1.75 x 10^{9} L$^{0.5}$ mol$^{-0.5}$ s^{-1} and the activation energy is 35.7 kcal mol^{-1}. The heat capacities of A, B, Y, and Z are 37, 34, 36, and 38 cal mol^{-1} K^{-1}, respectively. If an adiabatic 5.0 L BSTR is charged with equal molar amounts of A and B at 400 °C and 1 atm, how long will it take to convert 50% of reagent A and what will the temperature equal?

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: adiabatic, gas-phase BSTR

Given Constants: ΔH_1 = –12.9 kcal mol^{-1}, $k_{0,1}$ = 1.75 x 10^{9} L$^{0.5}$ mol$^{-0.5}$ s^{-1}, E_1 = 35.7 kcal mol^{-1}, $\hat{C}_{p,A}$ = 37 cal mol^{-1} K^{-1}, $\hat{C}_{p,B}$ = 34 cal mol^{-1} K^{-1}, $\hat{C}_{p,Y}$ = 36 cal mol^{-1} K^{-1}, $\hat{C}_{p,Z}$ = 38 cal mol^{-1} K^{-1}, V = 5.0 L, $y_{A,0}$ = 0.5, $y_{B,0}$ = 0.5, T_0 = 400 °C, P_0 = 1 atm, and f_A = 0.5.

Deliverables: t_f and T_f

Formulation of the Equations

Reactor Model Equations:

$$\frac{dn_A}{dt} = -\, r_1 V \qquad (3)$$

$$\frac{dn_B}{dt} = -\, r_1 V \qquad (4)$$

$$\frac{dn_Y}{dt} = r_1 V \qquad (5)$$

$$\frac{dn_Z}{dt} = r_1 V \qquad (6)$$

$$\left(n_A \hat{C}_{p,A} + n_B \hat{C}_{p,B} + n_Y \hat{C}_{p,Y} + n_Z \hat{C}_{p,Z}\right) \frac{dT}{dt} - V \frac{dP}{dt} = -\, r_1 V \Delta H_1 \qquad (7)$$

$$RT\left(\frac{dn_A}{dt} + \frac{dn_B}{dt} + \frac{dn_Y}{dt} + \frac{dn_Z}{dt}\right) + \left(n_A + n_B + n_Y + n_z\right) R \frac{dT}{dt} - V \frac{dP}{dt} = 0 \qquad (8)$$

Reactor Model Variables: $\underline{t}$, $\underline{n}_A$, $\underline{n}_B$, $\underline{n}_Y$, $\underline{n}_Z$, $\underline{T}$, and $\underline{P}$

Additional Computable Unknowns: r_1, k_1, C_A, C_B

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \qquad (9)$$

$$C_i = \frac{n_i}{V} \qquad i = A \text{ and } B \qquad (10)$$

IVODE Solver Inputs:

1. Initial values of the reactor model variables shown in Table 1.

2. Stopping criterion that n_A equals the final value shown in Table 1.
3. Derivatives function that
   a. receives the BSTR model variables at the start of an integration step
   b. returns the corresponding BSTR derivatives

$$\boldsymbol{M} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sum_i \left(n_i \hat{C}_{p,i} \right) & -V \\ RT & RT & RT & RT & R \sum_i n_i & -V \end{bmatrix} \tag{11}$$

$$\underline{g} = \begin{bmatrix} -Vr_1 \\ -Vr_1 \\ Vr_1 \\ Vr_1 \\ -Vr_1 \Delta H_1 \\ 0 \end{bmatrix} \tag{12}$$

$$\begin{bmatrix} \frac{dn_A}{dt} \\ \frac{dn_B}{dt} \\ \frac{n_Y}{dt} \\ \frac{n_Z}{dt} \\ \frac{dT}{dt} \\ \frac{dP}{dt} \end{bmatrix} = \boldsymbol{M}^{-1} \underline{g} \tag{13}$$

Table 1. Initial and final values of the design equation variables.

Variable	Initial Value	Final Value
t	0	
n_A	$n_{A,0} = \dfrac{P_0 V}{R T_0}$	$n_{A,f} = n_{A,0}\left(1 - f_A\right)$
n_Y	0	
n_Z	0	
T	T_0	
P	P_0	

Implementation of the Calculations

The Python script, practice_17.py, that was written to perform the calculations accompanies this solution. It defines a BSTR model function and derivatives function that solve the BSTR design equations, which is all that needs to be done.

Results, Discussion

The calculations were performed as described. Reaching 50% conversion requires 7.2 min and results in a temperature of 490 °C. The calculations were checked by noting that the reaction does not affect the total number of moles and the volume is constant, so the pressure depends only on the temperature. Solving the design equations yields the final pressure, and it can be calculated using the ideal gas law and the final temperature. Both calculations yielded the same value for the final pressure, 1.13 atm.

Deliverables

Reaching 50% conversion requires 7.2 min and results in a temperature of 490 °C.