REB, The Course
Class 14 Learning Activity Solution

Liquid phase reaction (1) takes place in an adiabatic batch reactor with a volume of 1200 L. The reactor initially contains 2500 mol of A and 50,000 moles of B at a temperature of 300K. The reaction is allowed to proceed until half of the A has been consumed. The rate expression is given in equation (2) where the pre-exponential factor equals 6 x 10^5 min^{-1} and the activation energy is 42 kJ mol^{-1}. If the heat capacities of A, B and Z are constant and equal to 180, 70 and 225 J mol^{-1} K^{-1}, respectively, and the heat of reaction at 298 K is equal to –16.5 kJ mol^{-1}, how long will the reaction run and what will be the final temperature?

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

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

Assignment Summary

<u>Reaction</u>

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

<u>Rate Expression</u>

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

<u>Reactor</u>: Adiabatic, liquid-phase BSTR with a one step operating protocol

<u>Given Constants</u>: V = 1200 L, $n_{A,0}$ = 2500 mol, $n_{B,0}$ = 50,000 mol, T_0 = 300K, $f_{A,f}$ = .0.5, $k_{0,1}$ = 6 x 10^5 min^{-1}, E_1 = 42 kJ mol^{-1}, $\hat{C}_{p,A}$ = 180 J mol^{-1} K^{-1}, $\hat{C}_{p,B}$ = 70, $\hat{C}_{p,Z}$ = 225 J mol^{-1} K^{-1}, and $\Delta H_1^0\Big|_{298\,K}$ = –16.5 kJ mol^{-1}.

<u>Deliverables</u>: t_f and T_f.

Formulation of the Equations

<u>Reactor Model Equations</u>:

$$\frac{dn_A}{dt} = -Vr_1 \tag{3}$$

$$\frac{dn_B}{dt} = -Vr_1 \tag{4}$$

$$\frac{dn_Z}{dt} = Vr_1 \tag{5}$$

$$\frac{dT}{dt} = \frac{-Vr_1 \Delta H_1}{n_A \hat{C}_{p,A} + n_B \hat{C}_{p,B} + n_Z \hat{C}_{p,Z}} \tag{6}$$

<u>Reactor Model Variables</u>: $\underline{t}$, $\underline{n}_A$, $\underline{n}_B$, $\underline{n}_Z$, and $\underline{T}$

<u>Additional Computable Unknowns</u>: r_1, k_1, C_A, and ΔH_1

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \tag{7}$$

$$C_A = \frac{n_A}{V} \tag{8}$$

$$\Delta H_1 = \Delta H_1^0\Big|_{298\,K} + \left(\hat{C}_{p,Z} - \hat{C}_{p,A} - \hat{C}_{p,B}\right)(T - 298\,K) \tag{9}$$

<u>IVODE Solver Inputs</u>:

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. Residuals/Derivatives function that
   a. receives the independent and dependent variables (t, n_A, n_B, n_Z, and T) at the start of an integration step
   b. returns the corresponding reactor model derivatives (equations (3) through (6))

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

Variable	Initial Value	Final Value
t	0	
n_A	$n_{A,0}$	$n_{A,f} = n_{A,0}\left(1 - f_{A,f}\right)$
n_B	$n_{B,0}$	
n_Z	0	
T	T_0	

<u>Deliverables Equations</u>:

$$t_f = \underline{t}\,\big|_{n_A=n_{A,f}} \tag{10}$$

$$T_f = \underline{T}\,\big|_{n_A=n_{A,f}} \tag{11}$$

Implementation of the Calculations

The Python script, activity_14.py, that was written to perform the calculations accompanies this solution. Basically it defines a BSTR model function and a BSTR derivatives function that solve the BSTR design equations (3) through (6). After using them to solve the BSTR design equations, the deliverables are calculated, reported, and saved.

Results and Discussion

The calculations were performed as described above. The conversion reaches 45% in 20.2 min, at which time the reacting fluid temperature is 305 K. The increase in temperature is expected because the reaction is exothermic and the reactor operates adiabatically. The temperature rise is very small, however. This is likely because the heat of reaction is quite low, and the heat capacities are large.

In Example 7.4.1 of “Reaction Engineering Basics,” a similar system is examined. The qualitative analysis of the results notes that as the reaction progresses, the effect of decreasing reactant concentration opposes the effect of increasing temperature. In that example, the temperature effect predominates initially, but over time the concentration effect becomes larger. This results in the rate going through a maximum, and the discussion notes that such behavior is typical.

Here, given the very low temperature increase, it is possible that the concentration effect predominates at all times and the rate does not go through a maximum. To see whether that is true, the instantaneous rate was calculated and is plotted versus reaction time in Figure 1. Indeed, the rate does not pass through a maximum here, but simply decreases monotonically.

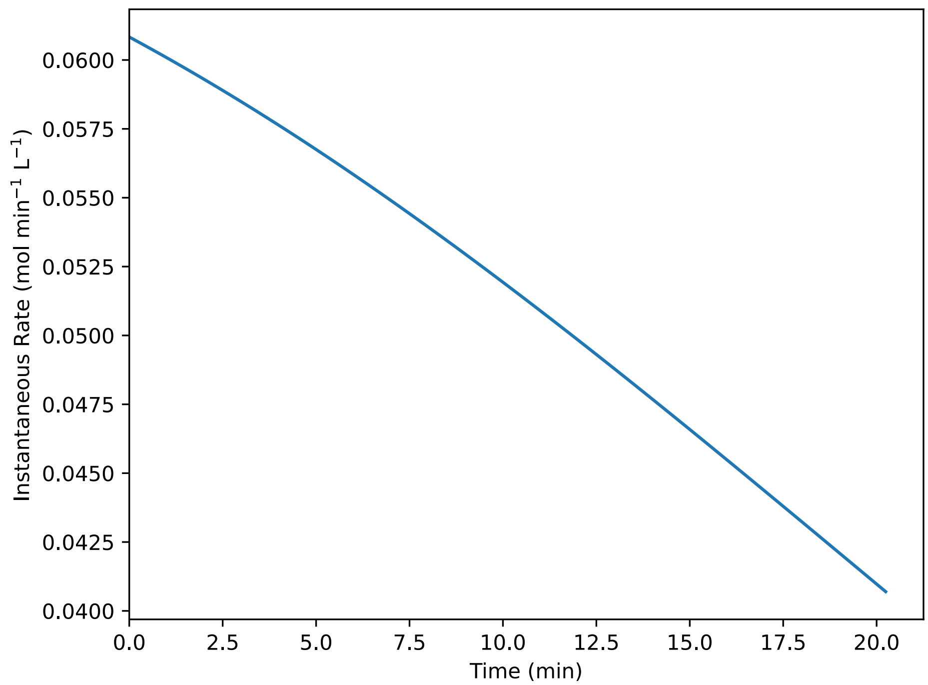

Figure 1. Instantaneous reaction rate as a function of reaction time.

Deliverables

The conversion reaches 45% in 20.2 min, at which time the reacting fluid temperature is 305 K.