REB, The Course
Class 12 Practice Assignment Solution

Liquid phase reaction (1) takes place in an adiabatic CSTR with a volume of 1.5 L operating at atmospheric pressure. The 50 °C feed to the reactor is 1.5 M in A and 2.5 M in B. The kinetics are given by equation (2) with k_0 = 1.4 x 10^{14} min^{-1} and E = 22 kcal mol^{-1}. The heat of reaction is –211 kJ mol^{-1}, and the heat capacity of the fluid is 1.3 cal cm^{-3} K^{-1}. The reactor is going to be started up at a space time of 10 min by initially filling it with solvent (no reactants or products) at 50 °C and then starting the feed flow. Calculate and plot the outlet molar flow of Y and the outlet temperature as functions of time.

$$2\,A + B \rightleftarrows 2\,Y + 2\,Z \tag{1}$$

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

Assignment Summary

Reaction

$$2\,A + B \rightleftarrows 2\,Y + 2\,Z \tag{1}$$

Rate Expression

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

Reactor: liquid-phase, adiabatic, transient CSTR

Given Constants: V = 1.5 L, T_{in} = 50 °C, $C_{A,in}$ = 1.5 M, $C_{B,in}$ = 2.5 M, $k_{0,1}$ = 1.4 x 10^8 min^{-1}, E_1 = 30 kcal mol^{-1}, ΔH_1 = –211 kJ mol^{-1}, $\breve{C}_p$ = 1.3 cal cm^{-3} K^{-1}, τ = 10 min, and T_0 = 50 °C.

Deliverables: $\underline{\dot{n}_Y}$ vs. $\underline{t}$ and $\underline{T}$ vs. $\underline{t}$ as graphs

Formulation of the Equations

Reactor Model Equations:

$$\frac{d\dot{n}_A}{dt} = \frac{\dot{V}}{V}\left(\dot{n}_{A,in} - 2r_1V - \dot{n}_A\right) \tag{3}$$

$$\frac{d\dot{n}_B}{dt} = \frac{\dot{V}}{V}\left(\dot{n}_{B,in} - r_1V - \dot{n}_B\right) \tag{4}$$

$$\frac{d\dot{n}_Y}{dt} = \frac{\dot{V}}{V}\left(2r_1V - \dot{n}_Y\right) \tag{5}$$

$$\frac{d\dot{n}_Z}{dt} = \frac{\dot{V}}{V}\left(2r_1V - \dot{n}_Z\right) \tag{6}$$

$$\frac{dT}{dt} = -\frac{\dot{V}\breve{C}_p\left(T - T_0\right) + r_1V\Delta H_1}{V\breve{C}_p} \tag{7}$$

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

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

$$\dot{V} = \dot{V}_{in} \tag{8}$$

$$\dot{V}_{in} = \frac{V}{\tau} \tag{9}$$

$$\dot{n}_{i,in} = \dot{V}_{in}C_{i,in} \qquad i = A \text{ and } B \tag{10}$$

$$k_1 = k_{0,1}\exp\left(\frac{-E_1}{RT}\right) \tag{11}$$

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{12}$$

IVODE Solver Inputs:

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

2. Stopping criterion that t equals the final value shown in Table 1
3. Derivatives function that
   a. receives t, $\dot{n}_A$, $\dot{n}_B$, $\dot{n}_Y$, $\dot{n}_Z$, and T at the start of an integration step
   b. returns the corresponding reactor model derivatives

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

Variable	Initial Value	Final Value
t	0	t_f = 60 min
$\dot{n}_A$	0	
$\dot{n}_B$	0	
$\dot{n}_Y$	0	
$\dot{n}_Z$	0	
T	T_0	

Implementation of the Calculations

The Python script, practice_12.py, that was written to perform the calculations accompanies this solution.

Results and Discussion

The calculations were performed as described above. The outlet molar flow rate of reagent Y is plotted as a function of time in Figure 1, and the outlet temperature vs. time is plotted in Figure 2. Both quantities smoothly transition to their steady-state values in approximately 50 minutes.

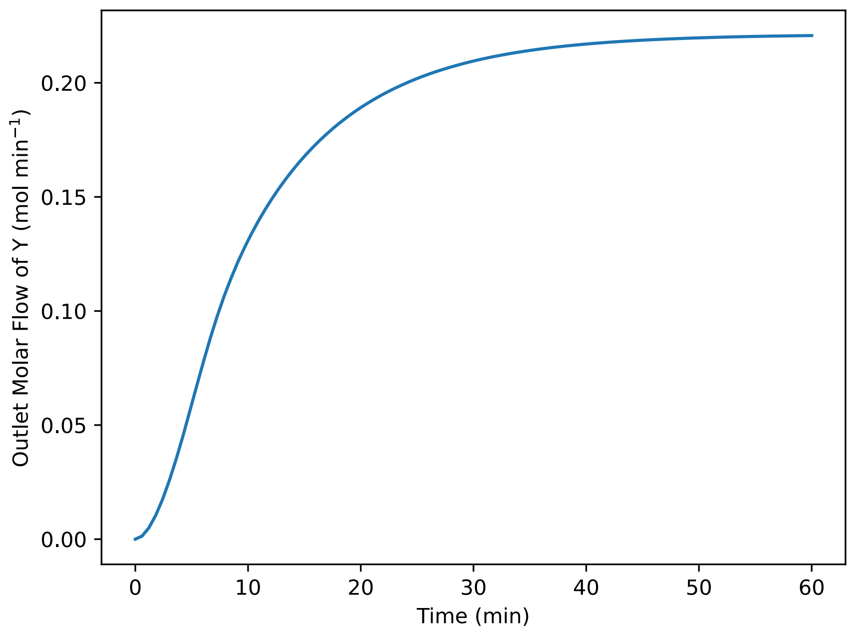

Figure 1. Outlet molar flow rate of reagent Y during CSTR startup.

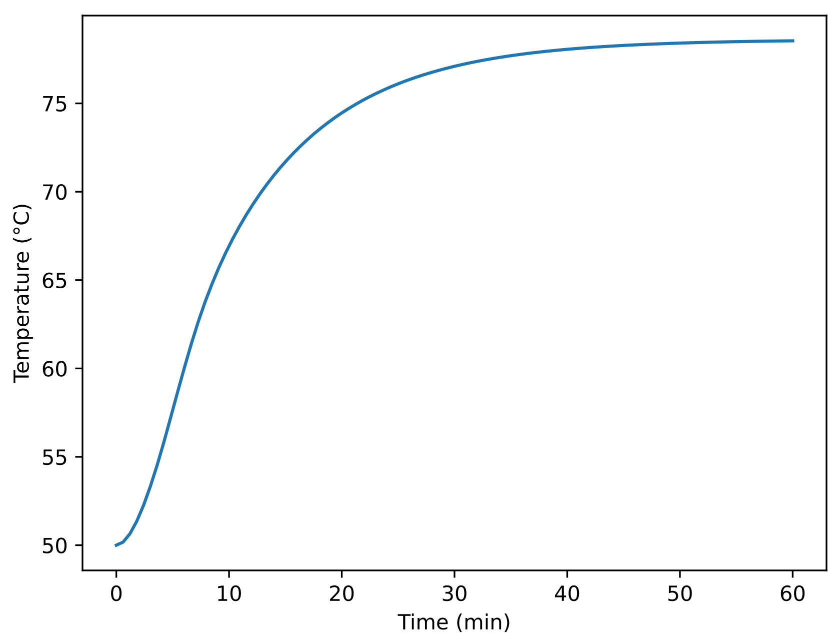

Figure 2. Outlet temperature during CSTR startup.

Before implementing this startup procedure the number of possible steady states should be determined to make sure the desired one is reached. Other startup procedures should also be investigated to see if the time required can be reduces without increasing costs.

Deliverables

The specified startup process reaches a steady state where the outlet flow of reagent Y is 0.22 mol min^{-1} and the temperature is 77 °C in approximately 50 minutes.