REB, The Course
Class 18 Practice Assignment Solution

An 11.5 L BSTR is charged with a 3.6 M liquid solution of reagent A at 35 °C. The reactor has a jacket with a volume of 1.4 L, a heat transfer area of 0.012 m^2, and a heat transfer coefficient of 1485 cal m^{-2} min^{-1} K^{-1}. Saturated steam at 1 atm (373.15 K) condenses in the jacket and exits as saturated water. The heat of vaporization of water at 1 atm and 373.15 K is 540 cal g^{-1}. Reaction (1) takes place within the BSTR; the rate expression is given in equation (2) where the forward and reverse rate display Arrhenius temperature dependence with $k_{0,f}$ = 6.297 x 10^5 L mol^{-1} min^{-1}, E_f = 12.65 kcal mol^{-1}, $k_{0,r}$ = 5.148 x 10^{18} L mol^{-1} min^{-1}, and E_r = 30.95 kcal mol^{-1}. The heat of reaction (1) is –18.3 kcal mol^{-1}. The reacting fluid density, 1.0 g L^{-1}, and heat capacity, 1.0 cal g^{-1} K^{-1}, are constant. Plot the conversion, reacting fluid temperature, and condensate mass flow rates during the first 2 h of operation.

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

$$r_1 = k_{1,f} C_A^2 - k_{1,r} C_Y C_Z \tag{2}$$

Assignment Summary

Reaction

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

Rate Expression

$$r_1 = k_{1,f} C_A^2 - k_{1,r} C_Y C_Z \tag{2}$$

Reactor: non-isothermal BSTR with a one-stage operating protocol

Given Constants: V = 11.5 L, $C_{A,0}$ = 3.6 M, T_0 = 35 °C, V_{ex} = 1.4 L, A = 0.012 m^2, U = 1485 cal m^{-2} min^{-1} K^{-1}, P_{ex} = 1 atm, T_{ex} = 373.15 K, $\Delta H_{vap,ex}$ = 540 cal g^{-1}, $k_{0,f}$ = 6.297

x 10^5 L mol^{-1} min^{-1}, E_f = 12.65 kcal mol^{-1}, $k_{0,r}$ = 5.148 x 10^{18} L mol^{-1} min^{-1}, E_r = 30.95 kcal mol^{-1}, ΔH_1 = –18.3 kcal mol^{-1}, ρ = 1.0 g L^{-1}, $\tilde{C}_p$ = 1.0 cal g^{-1} K^{-1}, and t_f = 2 h.

Deliverables: $\underline{f}_A$, $\underline{T}$, and $\underline{\dot{m}}_{cond}$ vs. $\underline{t}$ as graphs.

Formulation of the Equations

Reactor Model Equations:

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

$$\frac{dn_Y}{dt} = Vr_1 \tag{4}$$

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

$$\frac{dT}{dt} = \frac{\dot{Q} - Vr_1\Delta H_1}{V\rho\tilde{C}_p} \tag{6}$$

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

Additional Computable Unknowns: r_1, $k_{1,f}$, $k_{1,r}$, C_A, C_Y, C_Z, $\dot{Q}$

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

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

$$C_i = \frac{n_i}{V} \qquad i = A, Y, \text{ and } Z \tag{9}$$

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

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 the BSTR model variables at the start of an integration step
   b. calculates the additional computable unknowns
   c. evaluates and returns the BSTR design equation derivatives

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

Variable	Initial Value	Final Value
t	0	t_f
n_A	$n_{A,0} = C_{A,0}V$	
n_Y	0	
n_Z	0	
T	T_0	

Deliverables Equations:

$$\underline{f}_A = \frac{n_{A,0} - \underline{n}_A}{n_{A,0}} \tag{11}$$

$$\underline{\dot{m}}_{cond} = \frac{UA\left(T_{ex} - \underline{T}\right)}{\Delta H_{vap}} \tag{12}$$

Implementation of the Calculations

The Python script, practice_18.py, that was written to perform the calculations accompanies this solution. It defines a BSTR model function and a BSTR derivatives function that use an IVODE solver to solve the BSTR design equations. After solving the design equations, the conversion and condensate flow rates are calculated and the requested graphs are generated.

Results and Discussion

The calculations were performed as described above. Figure 1 shows the conversion during the first 2 hours of operation, Figure 2, the reacting fluid temperature, and Figure 3, the condensate mass flow rate. The conversion increases during the first 100 minutes after which it passes through a weak minimum and then decreases. The cause for this behavior is the combination of the reversibility of the reaction and the heat being added by the steam. The reaction is exothermic, and as a consequence, the equilibrium conversion decreases as the temperature increases. Thus, the reaction has effectively reached equilibrium at the point where the conversion is maximized. As the temperature continues to rise due to the steam heating, the reaction proceeds in the reverse direction so as to maintain equilibrium.

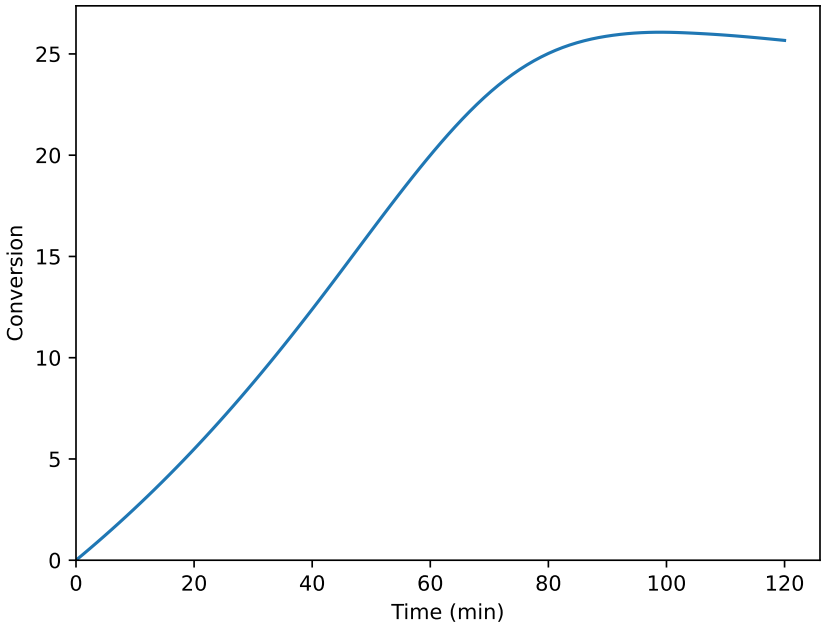

Figure 1. Conversion of A during the first 2 h of processing.

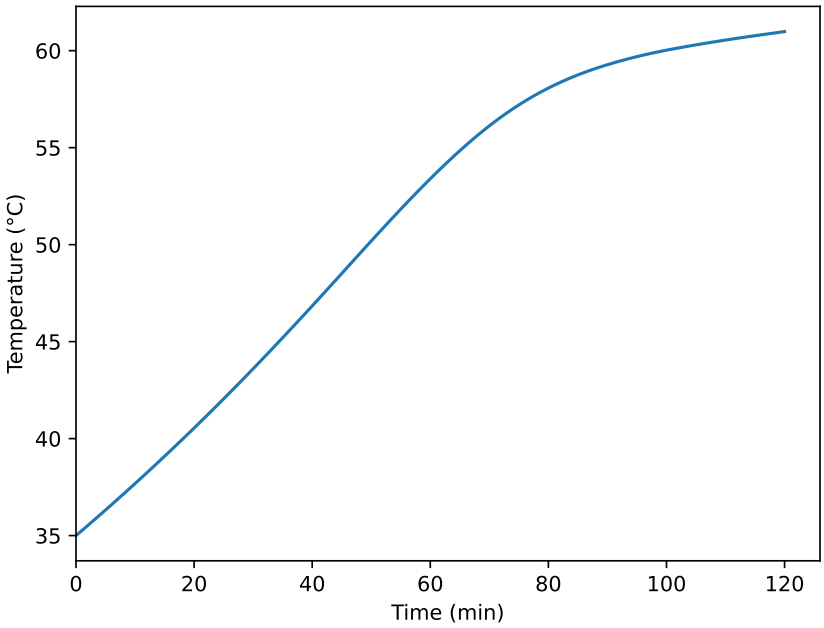

Figure 2. Reacting fluid temperature during the first 2 h of processing.

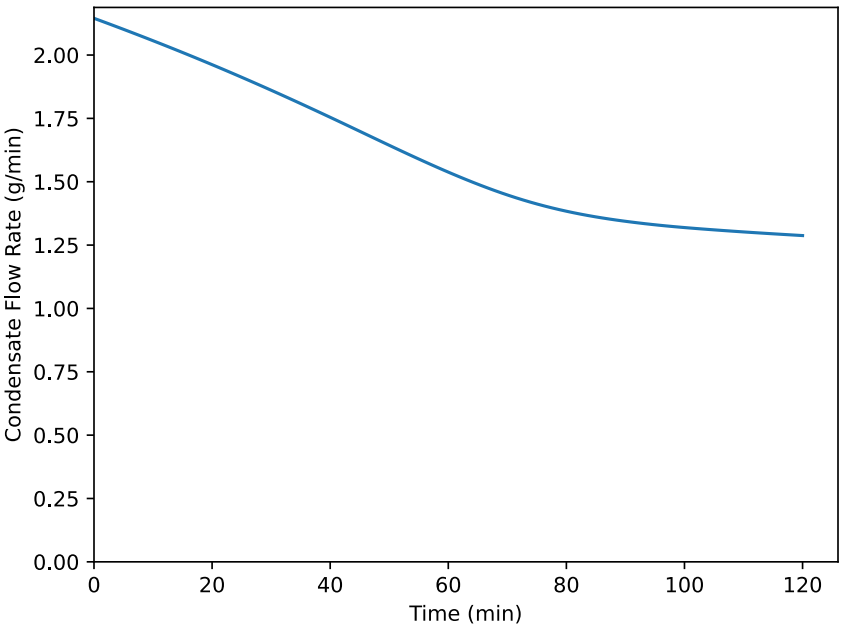

Figure 3. Condensate mass flow rate during the first 2 h of processing.

Figure 1 shows that the rate of increase of the conversion is significant even at the start of the process. This suggests that it might be possible to operate the reactor adiabatically. Doing so would decrease the rate of temperature rise, so the conversion would increase less rapidly, but the conversion would simply become constant once equilibrium was reached. It would not pass through a maximum and decrease. It might prove advantageous to only use steam heating early in the process and then switch to adiabatic operation sometime before the maximum conversion is reached.

Deliverables

Figures 1 through 3 shown the conversion, reacting fluid temperature, and condensate mass flow rate during the first two hours of processing.