REB, The Course
Class 15 Learning Activity Solution

A batch stirred tank reactor is being used for the production of Z according to reaction (1). Reactants A and B are available in separate 3 M solutions at 50 °C. To avoid undesirable side reactions, the reacting fluid must remain at or below 90 °C at all times. To facilitate doing so, the reactor has a cooling jacket with an area of 66 cm^2, a volume of 40 cm^3 and a heat transfer coefficient of 35 BTU ft^{-2} h^{-1} $°F^{-1}$. Cooling water is available at 40 °C. Turnaround time for the reactor is 30 min.

The heat capacity of all solutions containing A, B, Y and/or Z is essentially constant and equal to that of the solvent, 0.35 cal g^{-1} K^{-1}, and the density of all solutions is constant and equal to 0.93 g cm^{-3}. The rate expression for reaction (1) is given in equation (2) where the pre-exponential factor equals 1.24 x 10^{13} cm^3 mol^{-1} s^{-1} and the activation energy equals 20 kcal mol^{-1}. The heat of reaction (1) may be assumed to be constant and equal to -80 kJ mol^{-1}. The cooling water density and heat capacity may be assumed to equal 1 g cm^{-3} and 1 cal g^{-1} K^{-1}, respectively.

At the start of each batch, the reactor contains 250 cm^3 of the solution containing A and the jacket is full of water at 40 °C. To begin processing, 250 cm^3 of the solution containing B is instantaneously added, and cooling water flow is initiated. Processing ends when the conversion reaches 90%. Calculate the coolant flow rate at which the maximum reacting fluid temperature equals 90 °C. Then plot the net rate of production of Z as a function of reaction time when that cooling rate is used.

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: liquid-phase, non-isothermal BSTR

Given Constants: $C_{A,0}$ = 3 M, $C_{B,0}$ = 3 M, T_0 = 50 °C, T_{max} = 90 °C, A = 66 cm^2, V_{ex} = 40 cm^3, U = 35 BTU ft^{-2} h^{-1} °F$^{-1,}$ $T_{ex,in}$ = 40 °C, t_{turn} 30 min, $\tilde{C}_p$ = 0.35 cal g^{-1} K^{-1}, ρ = 0.93 g cm^{-3}, $k_{0,1}$ = 1.24 x 10^{13} cm^3 mol^{-1} s^{-1}, E_1 = 20 kcal mol^{-1}ΔH_1 = –80 kJ mol-$^{-1}$, ρ_{ex} = 1 g cm^{-3}, $\tilde{C}_{p,ex}$ = 1 cal g^{-1} K^{-1}, $V_{A,0}$ = 250 cm^3, $T_{ex,0}$ = 40 °C, $V_{B,0}$ = 250 cm^3, and f_A = 90%.

Deliverables: $\dot{m}_{ex}$, $\underline{r}_{net,Z}$ vs. $\underline{t}$ as a graph

Formulation of the Equations

Reactor Model Equations:

$$\frac{dn_A}{dt} = -r_1 V \tag{3}$$

$$\frac{dn_B}{dt} = -r_1 V \tag{4}$$

$$\frac{dn_Y}{dt} = r_1 V \tag{5}$$

$$\frac{dn_Z}{dt} = r_1 V \tag{6}$$

$$\frac{dT}{dt} = \frac{\dot{Q} - Vr_1\Delta H_1}{\rho V\tilde{C}_p} \tag{7}$$

$$\frac{dT_{ex}}{dt} = \frac{-\dot{Q} - \dot{m}_{ex}\tilde{C}_{p,ex}\left(T_{ex} - T_{ex,in}\right)}{\rho_{ex}\tilde{C}_{p,ex}V_{ex}} \tag{8}$$

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

Additional Computable Unknowns: r_1, k_1, C_A, C_B, V, and $\dot{Q}$

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

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

$$V = V_{A,0} + V_{B,0} \tag{11}$$

$$\dot{Q} = UA\left(T_{ex} - T\right) \tag{12}$$

Additional Coupled Unknowns: $\dot{m}_{ex}$

$$\dot{m}_{ex} \ : \ \max\left(\underline{T}\right) = T_{max} \quad \Rightarrow \quad 0 = \max\left(\underline{T}\right) - T_{max} = \epsilon \tag{13}$$

ATE Solver Inputs:

1. Initial guesses for $\dot{m}_{ex}$
2. Residuals function that
    a. receives a guess for $\dot{m}_{ex}$
    b. solves the BSTR design equations using it
    c. uses that result to calculate and return ϵ

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. calculates the additional unknowns
   c. returns the corresponding values of the BSTR derivatives

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

Variable	**Initial Value**	**Final Value**
t	0	
n_A	$n_{A,0} = C_{A,0}V_{A,0}$	$n_{A,f} = n_{A,0}\left(1 - f_A\right)$
n_B	$n_{B,0} = C_{B,0}V_{B,0}$	
n_Y	0	
n_Z	0	
T	T_0	
T_{ex}	$T_{ex,0}$	

Deliverables Equations:

$$\underline{r}_{Z,net} = \frac{\underline{n}_Z}{\underline{t} + t_{turn}} \tag{14}$$

Implementation of the Calculations

The Python script, activity_15.py, that was written to perform the calculations accompanies this solution. It defines a BSTR model function and a BSTR derivatives function that solve the BSTR design equations, given a coolant mass flow rate. It also defines a coupled unknown residual function that calls the BSTR model function and uses the results to evaluate the coupled unknown residual. The calculations begin by defining a guess for the coolant mass flow rate. (The calculations converged with this guess; if they hadn't, a different guess would have needed to be defined.) Next an ATE solver is used to find the coolant mass flow rate, and then the result is used to solve the BSTR design equations. The net rate is calculated and the graph is generated.

Results and Discussion

The calculations were performed as described above. At a coolant mass flow rate of 56.4 g min^{-1} the maximum reacting fluid temperature will be 90 °C. At that coolant mass flow rate, the net rate will vary with reaction time as shown in Figure 1. The figure shows that the net rate reaches a maximum at a reaction time of ~13 min and then decreases slightly for the remainder of the process.

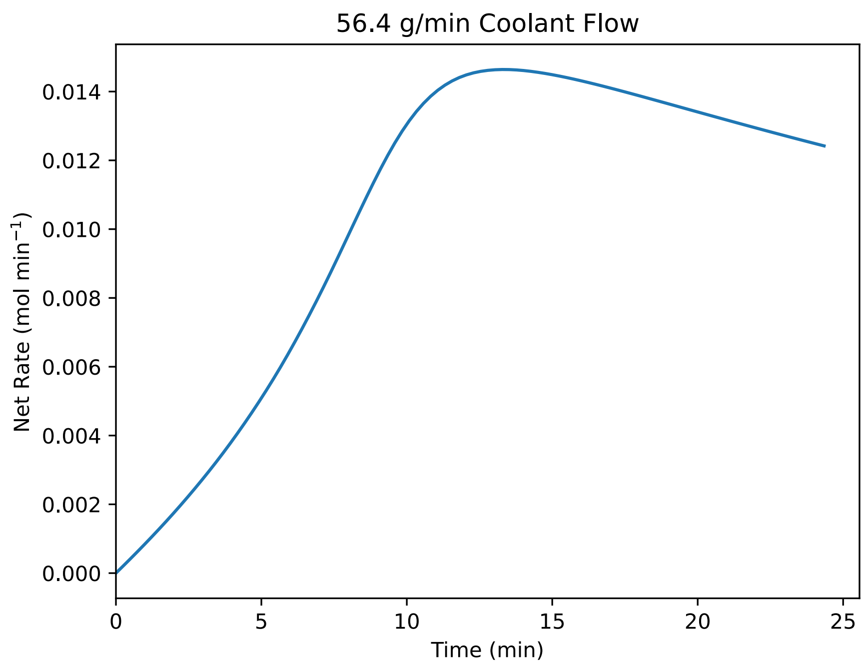

Figure 1. Net reaction rate profile at a coolant flow rate of 56.4 g min^{-1}.

At a fixed coolant inlet temperature, the coolant flow rate can be used to adjust the amount of heat removed from the reactor. As the coolant flow rate increases, the exit coolant temperature is expected to decrease. This creates a greater driving force for heat removal. The mean difference between the reacting fluid temperature and the coolant temperature increases.

Increasing the amount of heat removed by increasing the coolant flow rate can have two effects. First, for an exothermic reaction where the reacting fluid temperature is initially increasing, the maximum reacting fluid temperature will be reduced. However, if heat removal is increased too much, the reacting fluid may cool too fast. This can lead to a reduced rate and result in extremely long reaction times for reaching a given conversion.

To check that the maximum temperature in this example actually was 90 °C when the coolant flow rate was set to 56.4 g min^{-1}, The reacting fluid temperature was plotted as a function of reaction time. The calculations were then repeated using coolant mass flow rates slightly smaller (90% of the base value) and slightly larger (110% of the base value). The resulting temperature and net rate profiles are shown in Figures 2 and 3.

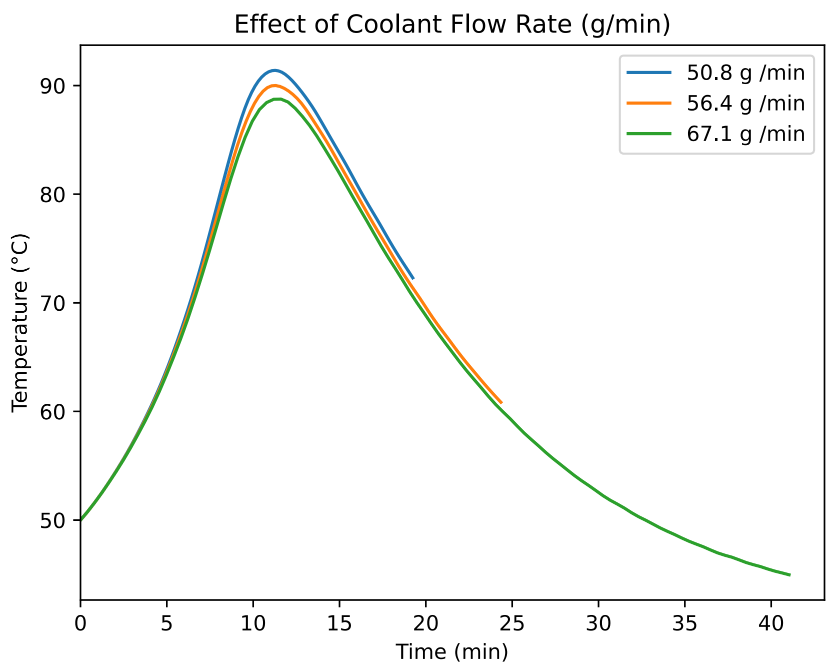

Figure 2. Effect of coolant mass flow rate on the temperature profile.

Figure 2 shows that (a) at a coolant flow rate of 56.4 g min^{-1}, the maximum temperature was indeed 90 °C, (b) that increasing the coolant flow rate did indeed reduce the maximum reacting fluid temperature, and (c) for the conditions used here, the reaction time did increase as the coolant flow rate increased, but not to an exorbitant degree. Figure 3 shows that after the maximum temperature (and net rate) was reached, the net rate did decrease steadily, but it did not rapidly fall to zero as it might have if the cooling was excessive.

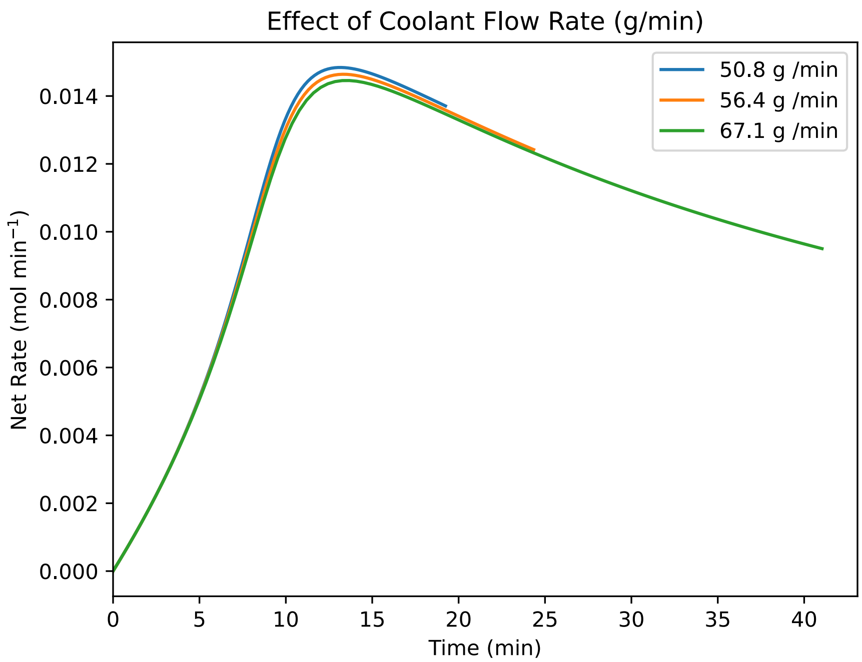

Figure 3. Effect of coolant flow rate on the net reaction rate.

Figures 2 and 3 highlight a trade-off associated with BSTRs. Here the final conversion was 90%, but the maximum net rate occurs well before that conversion is reached. Thus, operating at the maximum net rate reduces the conversion, but operating at high conversion reduces the net rate. This is one of the issues an engineer will face when designing a BSTR. The deciding factor in the trade-off between net rate and conversion likely will be financial and not technical.

Deliverables

A coolant mass flow rate of 56.4 g min^{-1} leads to a maximum reacting fluid temperature of 90 °C and the net rate profile shown in Figure 1.