REB, The Course
Class 10 Practice Assignmen Solution

A 4 L CSTR is being used to convert A to Z according to reaction (1). The rate expression for reaction (1) is given in equation (2). The rate coefficient obeys the Arrhenius expression with a pre-exponential factor equal to 2.59 x 10^9 min^{-1} and an activation energy equal to 16,500 cal mol^{-1}. The heat of reaction (1) may be taken to be constant and equal to –22,200 cal mol^{-1}. The heat capacity of the reacting solution is approximately constant and equal to 440 cal L^{-1} K^{-1}, and its density is constant. The reactor has a jacket with a volume of 0.5 L, a heat transfer area of 0.6 ft^2 and a heat transfer coefficient of 5.65 x 10^3 cal ft^{-2} h^{-1} K^{-1}. The cooling water may be taken to have a constant density of 1 g cm^{-3} and a constant heat capacity of 1 cal g^{-1} K^{-1}.

The feed is a solution containing only A at a concentration of 2M and a temperature of 60 °C, and cooling water at 20 °C flows into the jacket at 0.2 kg min^{-1}. Compare the conversion, outlet temperature, and outlet coolant temperature for space times of 50 and 60 min.

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: liquid-phase, steady-state, non-isothermal CSTR

Given Constants: V = 4 L, $k_{0,1}$ = 2.59 x 10^9 min^{-1}, E_1 = 16,500 cal mol^{-1}, ΔH_1 = –22,200 cal mol^{-1}, $\breve{C}_p$ = 440 cal L^{-1} K^{-1}, V_{ex} = 0.5 L, A = 0.6 ft^2, U = 5.65 x 10^3 cal ft^{-2} h^{-1}

K^{-1}, ρ_{ex} = 1 g cm^{-3}, $\tilde{C}_{p,ex}$ = 1 cal g^{-1} K^{-1}, $C_{A,in}$ = 2M, T_{in} = 60 °C, $T_{ex,in}$ = 20 °C, and $\dot{m}_{ex}$ = 0.2 kg min^{-1}.

<u>Parameter</u>: $\tau = [50, 60]$ min

<u>Deliverables</u>: f_A, T, and T_{ex} for each space time

Formulation of the Equations

<u>Reactor Model Equations</u>:

$$0 = \dot{n}_{A,in} - \dot{n}_A - r_1 V = \epsilon_1 \tag{3}$$

$$0 = -\dot{n}_Z + r_1 V = \epsilon_2 \tag{4}$$

$$0 = \dot{V}_{in} \breve{C}_p \left(T - T_{in}\right) + r_1 \Delta H_1 V - \dot{Q} = \epsilon_3 \tag{5}$$

$$0 = -\dot{m}_{ex} \tilde{C}_{p,ex} \left(T_{ex} - T_{ex,in}\right) - \dot{Q} = \epsilon_4 \tag{6}$$

<u>Reactor Model Variables</u>: $\dot{n}_A$, $\dot{n}_Z$, T, and T_{ex}

<u>Additional Computable Unknowns</u>: $\dot{n}_{A,in}$, $\dot{V}_{in}$, r_1, k_1, C_A, $\dot{V}$, and $\dot{Q}$

$$\dot{n}_{A,in} = \dot{V}_{in} C_{A,in} \tag{7}$$

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

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

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{10}$$

$$\dot{V} = \dot{V}_{in} \tag{11}$$

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

Additional Uncomputable Unknown: τ

$$\underline{\tau} \text{ min} \tag{13}$$

ATE Solver Inputs:

1. Initial guesses for the reactor model variables

$$\forall \tau_n \in \underline{\tau} \qquad \begin{pmatrix} \dot{V}_{in} = \frac{V}{\tau_n} \\ \dot{n}_{A,in} = C_{A,in}\dot{V}_{in} \\ \dot{n}_{A,guess} = \dot{n}_{A,in} \\ \dot{n}_{Z,guess} = 0 \\ T_{guess} = T_{in} + 5K \\ T_{ex,guess} = T_{ex} + 5K \end{pmatrix} \tag{14}$$

2. Residuals function that
   a. receives a guess for the reactor model variables
   b. returns the residuals corresponding to the reactor model equations

Deliverables Equations:

$$\forall \tau_n \in \underline{\tau} \qquad \begin{pmatrix} \dot{V}_{in} = \frac{V}{\tau_n} \\ \dot{n}_{A,in} = \dot{V}_{in}C_{A,in} \\ f_{A,n} = \frac{\dot{n}_{A,in} - \dot{n}_A\Big|_{\tau_n}}{\dot{n}_{A,in}} \\ T_n = T\Big|_{\tau_n} \\ T_{ex,in} = T_{ex}\Big|_{\tau_n} \end{pmatrix} \tag{18}$$

Implementation of the Calculations

The Python script, practice_10.py, that was written to perform the calculations accompanies this solution.

Results and Discussion

The calculations were performed as described above, and the results are shown in Table 1. The ATE solver converged using the initial guess in equation (18) for both space times. The results show that upon increasing the space time, the conversion, reacting fluid temperature, and exchange fluid temperature all decreased.

Table 1. Effect of space time on conversion, outlet temperature and coolant temperature.

Space Time (min)	Conversion (%)	T (°C)	Coolant T (°C)
50	86.2	76.4	32.4
60	81.7	69.0	30.8

In the absence of heat transfer, the conversion for an irreversible exothermic reaction would increase when the space time increased since the reactants have more time to react. Here, however the conversion decreases when the space time increases. The reason for this is that the reacting fluid has more time to react, and it has more time to transfer heat. If the increase in heat transfer to the heat exchange fluid due to that extra time is greater than the heat released by reaction, the temperature will decrease. The lower temperature leads to a lower rate, and consequently a lower conversion.

Furthermore, while the residence time of the reacting fluid is decreased, changing the space time does not change the amount of time the heat exchange fluid spends in the reactor jacket. Notice that not only is the reacting fluid temperature lower at the higher space time, but the exchange fluid temperature is also lower at the higher space time. This makes sense because the coolant spends the same amount of time in the shell, but less heat needs to be removed due to the lower reaction rate. Consequently, the coolant temperature does not increase as much as at the lower space time.

Deliverables

The conversion, reacting fluid temperature, and exchange fluid temperature at space times of 50 and 60 min are shown in Table 1.