# REB, The Course
# Class 19 Practice Assignment Solution

Acid A is to be neutralized using base B, reaction (1), by slowly adding a 4 M solution of the base to a 10 M solution of the acid. The neutralization reaction, (1) is irreversible with a heat of reaction equal to –44 kcal $mol^{-1}$. The reaction is first order in both acid and base with a pre–exponential factor of 8.11 x $10^{12}$ L $mol^{-1}$ $s^{-1}$ and an activation energy of 17.7 kcal $mol^{-1}$. A jacketed, perfectly mixed, reactor will be charged with 4 L of the 10 M solution of A at 20 °C, while cooling water at 20 °C flows at 1.0 kg $min^{-1}$ to the perfectly mixed, 0.5 L jacket. The heat transfer area is 0.6 $ft^2$ and the heat transfer coefficient is 1.13 x $10^4$ cal $ft^{-2}$ $h^{-1}$ $K^{-1}$. The cooling water and the solutions of A and B 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 pressure in the reactor will be constant and equal to 1 atm. Plot the acid concentration and the reactor temperature as a function of time if 10 L of the base solution at 20 °C is added at a rate of 0.05 L $min^{-1}$. Compare the results to those from the Class 14 Practice Assignment where the reactor was operated as a BSTR.

$$A + B \rightarrow S + H_2O \tag{1}$$

---

***Assignment Summary***

To simplify the notation, W is used here to represent $H_2O$.

Reaction

$$A + B \rightarrow S + H_2O \tag{1}$$

Rate Expression

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

Reactor: Single-stage, liquid-phase, cooled SBSTR

Given Constants: $C_{B,0}$ = 4 M, $C_{A,0}$ = 10 M, $\Delta H$ = –44 kcal mol$^{-1}$, $k_0$ = 8.11 x 10$^{12}$ L mol$^{-1}$ s$^{-1}$, $E$ = 17.1 kcal mol$^{-1}$, $V_{A,0}$ = 4 L, $T_0$ = 20 °C, $T_{ex,0}$ = 20 °C, $T_{ex,in}$ = 20 °C, $\dot{m}_{ex}$ = 1.0 kg min$^{-1}$, $V_{ex}$ = 0.5 L, $A_{ex}$ = 0.6 ft$^2$, $U$ = 1.13 x 10$^4$ cal ft$^{-2}$ h$^{-1}$ K$^{-1}$, $\rho$ = $\rho_{ex}$ = 1 g cm$^{-3}$, $\tilde{C}_p$ = $\tilde{C}_{p,ex}$ = 1.0 cal g$^{-1}$ K$^{-1}$, $P$ = 1 atm, $V_{B,0}$ = 10 L, $T_{in}$ = 20 °C, and $\dot{V}_{in}$ = 0.05 L min$^{-1}$.

Deliverables: $\underline{C_A}$ and $\underline{T}$ vs. $\underline{t}$ as graphs

***Formulation of the Equations***

Reactor Model Equations:

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

$$\frac{dn_B}{dt} = \dot{n}_{B,in} - Vr_1 \tag{4}$$

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

$$\frac{dn_W}{dt} = Vr_1 \tag{6}$$

$$V\tilde{C}_p\rho\frac{dT}{dt} - P\frac{dV}{dt} = \dot{Q} - \dot{V}_{in}\tilde{C}_p\rho\left(T - T_{in}\right) - Vr\Delta H \tag{7}$$

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

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

Reactor Model Variables: $\underline{t}$, $\underline{n_A}$, $\underline{n_B}$, $\underline{n_S}$, $\underline{n_W}$, $\underline{T}$, $\underline{T_{ex}}$, and $\underline{V}$

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

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \tag{10}$$

$$C_i = \frac{n_i}{V} \qquad i = A \text{ and } B \tag{11}$$

$$\dot{n}_{B,in} = \dot{V}_{in} C_{B,in} \tag{12}$$

$$\dot{Q} = UA_{ex}\left(T_{ex} - T\right) \tag{13}$$

IVODE Solver Inputs:

1. Initial values of the reactor model variables shown in Table 1
2. Stopping criterion that $V$ equals the final value shown in Table 1
3. Derivatives function that
   a. receives the reactor model variables at the start of an integration step
   b. calculates the additional computable unknowns, equations (10) - (13)
   c. evaluates and returns the design equation derivatives, equations (3) - (6), (14), (8) and (9)

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{V}_{in}\tilde{C}_p\rho\left(T - T_{in}\right) - Vr\Delta H + P\dot{V}_{in}}{V\tilde{C}_p\rho} \tag{14}$$

Table 1. Initial and final values of the BSTR model variables.

| Variable | Initial Value | Final Value |
|---|---|---|
| $t$ | 0 | |
| $n_A$ | $C_{A,0}V_{A,0}$ | |
| $n_B$ | 0 | |
| $n_S$ | 0 | |
| $n_W$ | 0 | |

| Variable | Initial Value | Final Value |
|---|---|---|
| $T$ | $T_0$ | |
| $T_{ex}$ | $T_{ex,0}$ | |
| $V$ | $V_{A,0}$ | $V_{A,0} + V_{B,0}$ |

Deliverables Equations:

$$\underline{C}_A = \frac{n_A}{V} \tag{15}$$

### *Implementation of the Calculations*

The Python script, practice_19.py, that was written to perform the calculations accompanies this solution. It defines an SBSTR model function and a derivatives function that solve the design equations using an IVODE solver. The calculations begin by using those functions to solve the design equations, after which the concentration of A during processing is calculated and the graphs are generated.

### *Results and Discussion*

The calculations were performed as described with no computational issues. The Class 14 Practice Assignment showed that in a BSTR the temperature would rise to 145.6 °C and the concentration of acid would drop to zero in less than 0.15 s. In other words, the reaction could not be controlled in a BSTR. The present results, shown in Figures 1 and 2, show that through the use of an SBSTR, the reaction can be controlled.

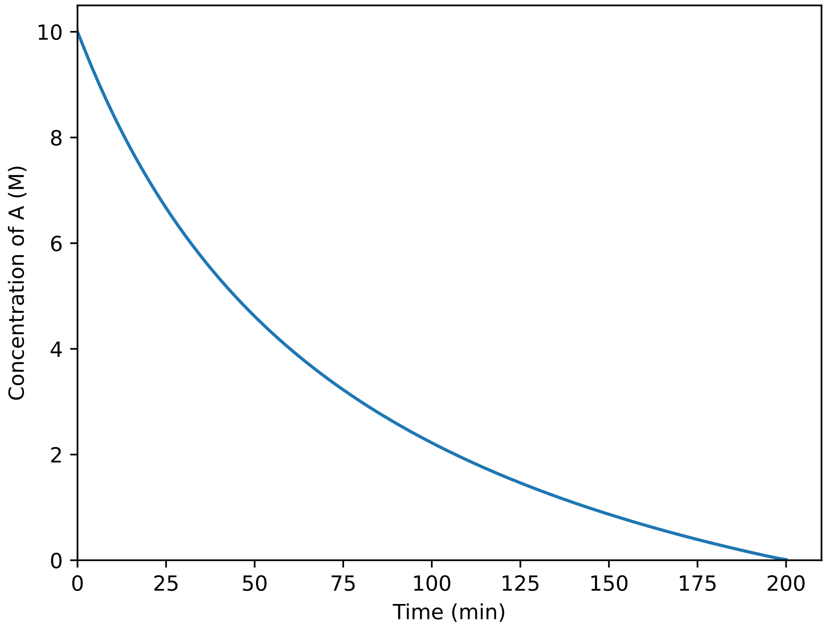


*Figure 1. Concentration of acid during semi-batch processing.*

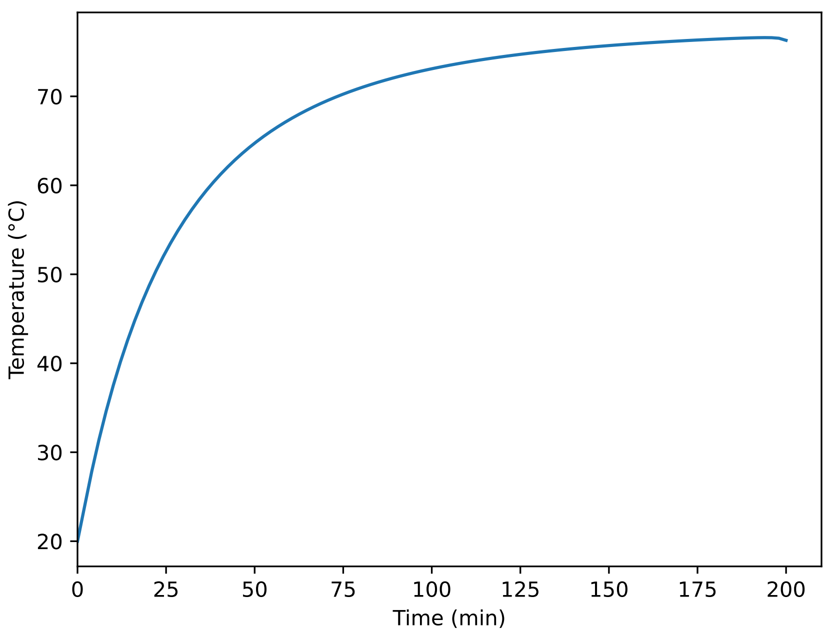


*Figure 2. Temperature during semi-batch processing.*

The previous results showed that the reaction is essentially instantaneous at these conditions. As a consequence, the rate of reaction, and therefore the rate of heat release, equals the rate at which B is fed to the reactor. In this example, neutralizing the acid required over three hours. That time could be shortened by adding the base more rapidly. The rate of addition should be matched to the heat removal capability of of the reactor.

### ***Deliverables***

The concentration of A and the reacting fluid temperature during SBSTR operation are shown in Figures 1 and 2, respectively.