REB, The Course
Class 14 Practice Assignment Solution

Acid A is to be neutralized using base B, reaction (1), by mixing a 4 M solution of the base with a 10 M solution of the acid. The neutralization reaction 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, 25 L batch 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. To start the reaction, 10 L of the 4 M solution of B at 20 °C will then added all at once. 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, the reactor temperature, and the exchange fluid temperature as functions of time after the addition of the base solution.

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

Assignment Summary

Reaction

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

Rate Expressions

$$r = kC_AC_B \tag{2}$$

Reactor: Liquid-phase, non-isothermal BSTR

Given Constants: $C_{B,0}$ = 4 M, $C_{A,0}$ = 10 M, ΔH = –44 kcal mol^{-1}, k_0 = 8.11 x 10^{12} L mol^{-1} s^{-1}, E = 17.1 kcal mol^{-1}, V = 25 L, $V_{A,0}$ = 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, $V_{B,0}$ = 10 L, A = 0.6 ft^2, U = 1.13 x 10^4 cal ft^{-2} h^{-1} K^{-1}, ρ = ρ_{ex} = 1 g cm^{-3}, $\tilde{C}_p$ = $\tilde{C}_{p,ex}$ = 1.0 cal g^{-1} K^{-1}, and P = 1 atm.

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

Formulation of the Equations

Reactor Model Equations:

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

$$\frac{dn_B}{dt} = -Vr \tag{4}$$

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

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

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

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

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

Additional Computable Unknowns: V, r, k, C_A, C_B, and $\dot{Q}$

$$V = V_{A,0} + V_{B,0} \tag{9}$$

$$k = k_0 \exp\left(\frac{-E}{RT}\right) \tag{10}$$

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

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

<u>IVODE Solver Inputs</u>:

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 independent and dependent variables (t, n_A, n_B, n_S, n_W, T, and T_{ex}) at the start of an integration step
   b. returns corresponding values of the BSTR design equation derivatives (equations (3) through (8))

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

Variable	Initial Value	Final Value
t	0	t_f = 10 min
n_A	$n_{A,0} = C_{A,0}V_{A,0}$	
n_B	$n_{B,0} = C_{B,0}V_{B,0}$	
n_S	0	
n_W	0	
T	T_0	
T_{ex}	$T_{ex,0}$	

<u>Deliverables Equations</u>:

$$\underline{C}_A = \frac{n_A}{V} \tag{13}$$

Implementation of the Calculations

The Python script, practice_14.py, that was written to perform the calculations accompanies this solution. It defines a BSTR function and a derivatives function that solve the design equations given a value for t_f. The calculations begin by setting t_f and then solving the design equations. The concentration of A versus time is calculated from the results, and the requested graphs are generated.

Results and Discussion

The variations of C_A, T, and T_{ex} over the first 10 minutes of processing are shown in Figures 1, 2, and 3. As might be expected, the figures show that the temperature rises very rapidly at the start of processing. The figure suggests it reaches ca. 145 °C, but it is likely that the reacting fluid would vaporize before that temperature was ever reached. The exchange fluid simply cannot remove the heat fast enough.

Clearly, a process like this would never actually be used. In Class 19 we will see how a semi-batch stirred tank reactor can be used instead of a BSTR to avoid the uncontrolled release of heat by the reaction.

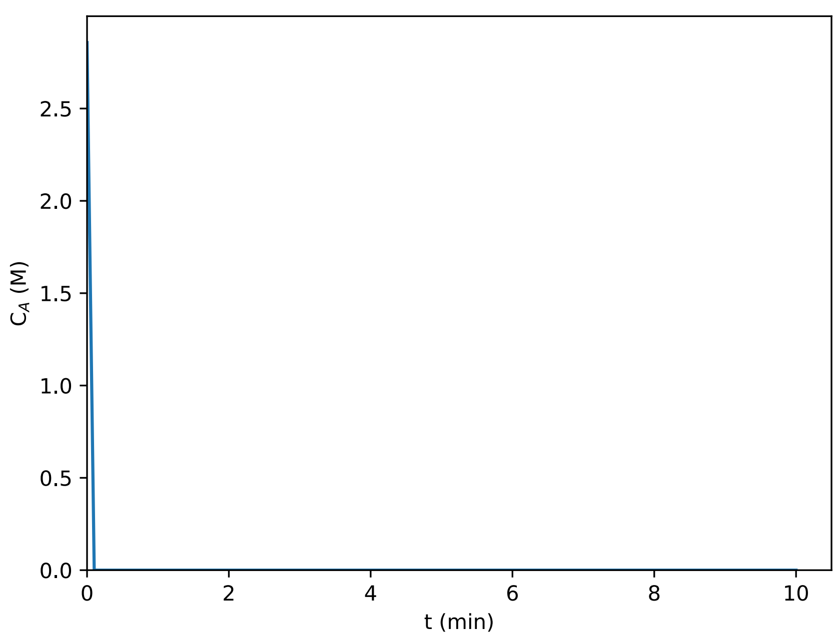

Figure 1: Variation in the concentration of the acid during the first 10 minutes of processing.

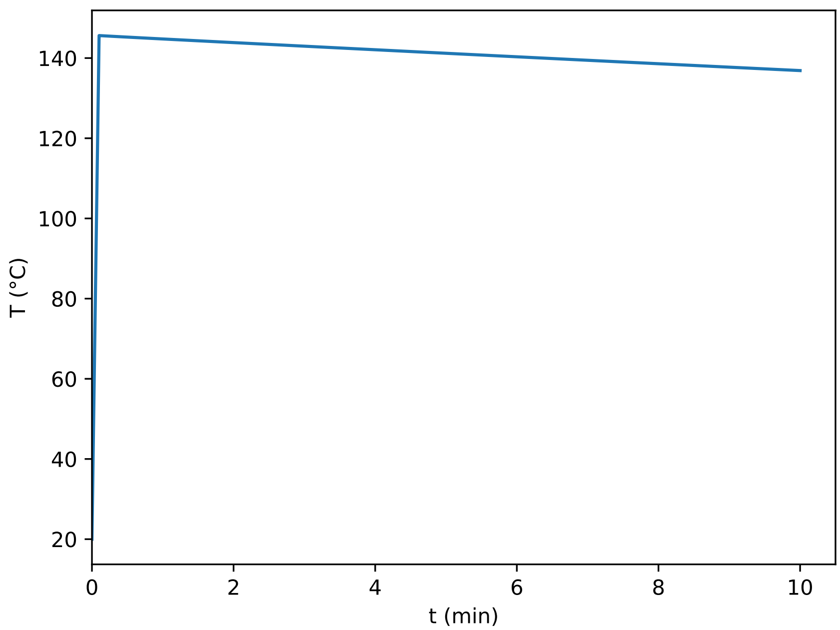

Figure 2: Variation of the reacting fluid temperature during the first 10 minutes of processing.

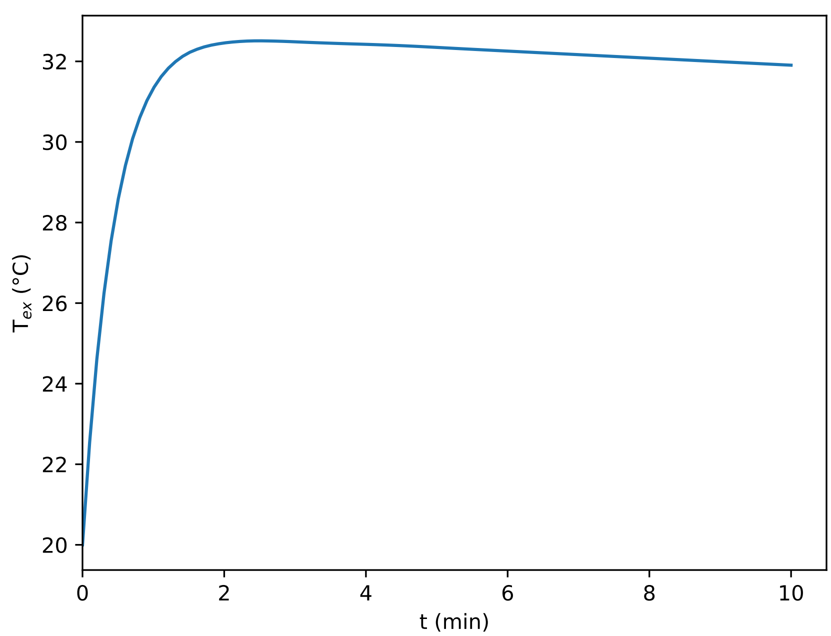

Figure 3: Variation of the exchange fluid temperature during the first 10 minutes of processing.

Deliverables

The variations of C_A, T, and T_{ex} over the first 10 minutes of processing are shown in Figures 1, 2, and 3.