REB, The Course
Class 13 Practice Assignment Solution

A jacketed, 17.7 ft^3 CSTR is operating at steady state. A liquid solution containing only reagent A at a concentration of 0.125 lbmol ft^{-3} is flowing into the reactor at 0.15 ft^3 min^{-1}, 300 °F, and 1 atm. The reacting solution is incompressible and has a constant heat capacity of 73.1 BTU ft^{-3} $°F^{-1}$. Reaction (1) is taking place within the CSTR at a rate given by equation (2) where the rate coefficient pre-exponential factor is 3.04 × 10^8 ft^3 $lbmol^{-1}$ min^{-1} and the activation energy is 29,100 BTU $lbmol^{-1}$. The heat of reaction is 32,800 BTU $lbmol^{-1}$ and is independent of temperature. A heat exchange fluid with a density of 81.2 lb_m ft^{-3} and a heat capacity of 1.06 BTU lb_m^{-1} $°F^{-1}$ flows into the jacket at 15 lb_m min^{-1} and 410 °F. The heat exchange fluid leaves the jacket at 355 °F. The jacket volume is 7 ft^3, the heat transfer area is 21.5 ft^2 and the overall heat transfer coefficient is equal to 1.71 BTU ft^{-2} min^{-1} $°F^{-1}$. The steady-state conversion of A is 85.3% and the steady-state outlet temperature is 332 °F. Suppose that an equipment failure elsewhere in the chemical plant caused the exchange fluid flow rate to instantaneously drop to a constant value of 5 lb_m min^{-1}. Plot the outlet concentration of Z and the reacting fluid temperature over the next 10 h assuming all other reactor inputs are unaffected.

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

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

Assignment Summary

<u>Reaction</u>

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

<u>Rate Expression</u>

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

<u>Reactor</u>: liquid-phase, non-isothermal, transient CSTR

Given Constants: V = 17.7 ft^3, $C_{A,in}$ = 0.125 lbmol ft^{-3}, $\dot{V}_{in}$ = 0.15 ft^3 min^{-1}, T_{in} = 300 °F, P = 1 atm, $\breve{C}_p$ = 73.1 BTU ft^{-3} °F^{-1}, $k_{0,1}$ = 3.04 × 10^8 ft^3 lbmol^{-1} min^{-1}, E_1 = 29,100 BTU lbmol^{-1}, ΔH_1 = 32,800 BTU lbmol^{-1}, ρ_{ex} = 81.2 lb ft^{-3}, $\tilde{C}_{p,ex}$ = 1.06 BTU lb$_m^{-1}$ °F^{-1}, $\dot{m}_{ex}$ = 5 lb$_m$ min^{-1}, $T_{ex,in}$ = 410 °F, $T_{ex,0}$ = 355 °F, V_{ex} = 7 ft^3, A = 21.5 ft^2, U = 1.71 BTU ft^{-2} min^{-1} °F^{-1}, $f_{A,0}$ = 85.3%, T_0 = 332 °F, and t_f = 10 h.

Deliverables: C_Z vs. t and T vs. t as graphs

Formulation of the Equations

Reactor Model Equations:

$$\frac{d\dot{n}_A}{dt} = \frac{\dot{V}}{V}\left(\dot{n}_{A,in} - \dot{n}_A - r_1 V\right) \tag{3}$$

$$\frac{d\dot{n}_Z}{dt} = \frac{\dot{V}}{V}\left(-\dot{n}_Z + r_1 V\right) \tag{4}$$

$$\frac{dT}{dt} = \frac{1}{V\breve{C}_p}\left(\dot{Q} - \dot{V}_0\breve{C}_p\left(T - T_{in}\right) - r_1 V \Delta H_1\right) \tag{5}$$

$$\frac{dT_{ex}}{dt} = \frac{1}{\rho_{ex}V_{ex}\tilde{C}_{p,ex}}\left(-\dot{Q} - \dot{m}_{ex}\tilde{C}_{p,ex}\left(T_{ex} - T_{ex,in}\right)\right) \tag{6}$$

Reactor Model Variables: t, $\dot{n}_A$, $\dot{n}_Z$, T, and T_{ex}

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

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

$$k_1 = k_{0,1}\exp\left(\frac{-E_1}{RT}\right) \tag{8}$$

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{9}$$

$$\dot{V} = \dot{V}_{in} \tag{10}$$

$$\dot{Q} = UA\left(T_{ex} - T\right) \tag{11}$$

IVODE Solver Inputs:

1. Initial values of the reactor model variables shown in Table 1
2. Stopping criterion that t equals the value shown in Table 1
3. Residuals/Derivatives function that
    a. receives the CSTR model variables (t, $\dot{n}_A$, $\dot{n}_Z$, T, and T_{ex})
    b. returns the corresponding values of the CSTR model derivatives

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

Variable	Initial Value	Final Value
t	0	t_f
$\dot{n}_A$	$\dot{n}_{A,in}\left(1 - f_{A,0}\right)$	
$\dot{n}_B$	$\dot{n}_{A,in} f_{A,0}$	
T	T_0	
T_{ex}	$T_{ex,0}$	

Deliverables Equations:

$$\underline{C}_Z = \frac{\dot{n}_Z}{\dot{V}} \tag{12}$$

Implementation of the Calculations

The Python script, practice_13.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 Figures 1 and 2.

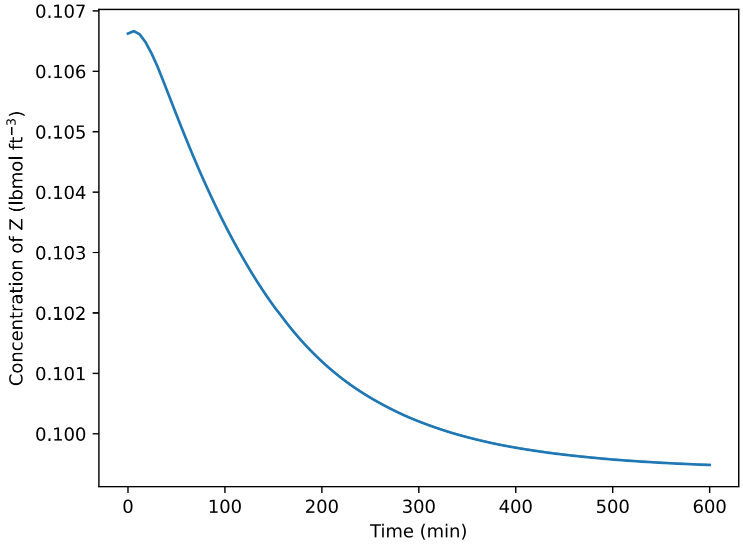

Figure 1. Outlet concentration of Y following a sudden decrease in the exchange fluid flow rate.

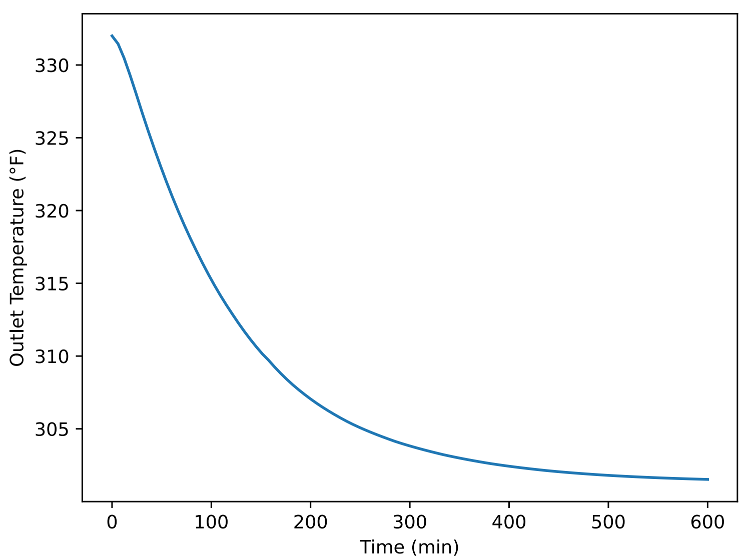

Figure 2. Outlet temperature following a sudden decrease in the exchange fluid flow rate.

The reaction is endothermic, and before the decrease in the heat exchange fluid flow rate, the outlet temperature of the reacting fluid was greater than the inlet temperature. This indicates that the exchange fluid was providing more heat than the reaction was absorbing. Figure 2 shows that after the exchange fluid flow decrease, the outlet reacting fluid temperature dropped close to its inlet value. This indicates that at the lower flow rate, the exchange fluid was only able to provide the heat that the reaction was absorbing.

As a consequence of the decrease in the reacting fluid temperature, the reaction rate will decrease. Because the reaction rate is lower, the concentration of the product, Y, leaving the reactor decreases as shown in Figure 1. After 10 h the reactor appears to have reached a new steady state where the concentration of Y is 0.095 lbmol ft^{-3} and the temperature is 302 °F.

Deliverables

After the heat exchange flow decreases, the outlet concentration of Y and the temperature both decrease as shown in Figures 1 and 2. After 10 h they appear to be approaching new steady state values of 0.095 lbmol ft^{-3} and 302 °F, respectively.