REB, The Book
Example 7.4.5 Solution

Liquid phase reactions (1) and (2) take place in a batch stirred-tank reactor; the reaction rate expressions are given in equations (3) and (4). The rate coefficients for reactions (1) and (2) obey the Arrhenius expression. For reaction (1) the pre-exponential factor is 1.6×10^{18} gal lbmol^{-1} h^{-1}, and the activation energy is 46,000 BTU lbmol^{-1}. For reaction (2) the pre-exponential factor is 4.5×10^{18} gal lbmol^{-1} h^{-1}, and the activation energy is 48,000 BTU lbmol^{-1}. The heat capacity of the reacting liquid is constant and equal to 65 BTU ft^{-3} °R^{-1}. The heat of reaction (1) is constant and equal to 45,000 BTU lbmol^{-1}, and the heat of reaction (2) is constant and equal to 39,500 BTU lbmol^{-1}. The 50 gal reactor initially contains only A and B at concentrations of 0.014 lbmol A gal^{-1} and 0.020 lbmol B gal^{-1}. The initial temperature of the reacting fluid is 70 °F. The reactor is jacketed with an overall heat transfer coefficient of 60 BTU ft^{-2} °R^{-1} h^{-1} and a heat transfer area of 13 ft^2. Saturated steam at 220 °F condenses in the jacket, leaving as a saturated liquid. (The heat of vaporization of steam at 220 °F is 966 BTU lb$_m^{-1}$.) Plot the yield of D (moles of D per initial mole of A), the temperature and the mass flow rate of water leaving the jacket as a function of the conversion of B.

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

$$D + B \rightarrow U + Z \tag{2}$$

$$r_1 = k_1 C_A C_B \tag{3}$$

$$r_2 = k_2 C_D C_B \tag{4}$$

Assignment Summary

Reactions

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

$$D + B \rightarrow U + Z \tag{2}$$

Rate Expressions

$$r_1 = k_1 C_A C_B \tag{3}$$

$$r_2 = k_2 C_D C_B \tag{4}$$

Reactor: liquid-phase, non-isothermal BSTR

Given Constants: $k_{0,1}$ = 1.6 × 10^{18} gal lbmol^{-1} h^{-1}, E_1 = 46,000 BTU lbmol^{-1}, $k_{0,2}$ = 4.5 × 10^{18} gal lbmol^{-1} h^{-1}, E_2 = 48,000 BTU lbmol^{-1}, $\breve{C}_p$ = 65 BTU ft^{-3} °R^{-1}, ΔH_1 = 45,000 BTU lbmol^{-1}, ΔH_2 = 39,500 BTU lbmol^{-1}, V = 50 gal, $C_{A,0}$ = 0.014 lbmol gal^{-1}, $C_{B,0}$ = 0.020 lbmol gal^{-1}, $C_{D,0} = C_{Z,0} = C_{U,0} = 0$, T_0 = 70 °F, U = 60 BTU ft^{-2} °R^{-1} h^{-1}, A = 13 ft^2, T_{ex} = 220 °F, and ΔH_{vap} = 966 BTU lb$_m^{-1}$.

Deliverables: $\underline{Y}_{D/A}$, $\underline{T}$, and $\underline{m}_{H_2O_{(l)}}$ vs. $\underline{f}_B$ as graphs

Reactor Model Equations:

$$\frac{dn_A}{dt} = -r_1 V \tag{5}$$

$$\frac{dn_B}{dt} = -\left(r_1 + r_2\right) V \tag{6}$$

$$\frac{dn_D}{dt} = \left(r_1 - r_2\right) V \tag{7}$$

$$\frac{dn_Z}{dt} = \left(r_1 + r_2\right) V \tag{8}$$

$$\frac{dn_U}{dt} = r_2 V \tag{9}$$

$$\frac{dT}{dt} = \frac{\dot{Q} - V\left(r_1 \Delta H_1 + r_2 \Delta H_2\right)}{V \breve{C}_p} \tag{10}$$

Reactor Model Variables: $\underline{t}$, $\underline{n}_A$, $\underline{n}_B$, $\underline{n}_D$, $\underline{n}_Z$, $\underline{n}_U$, and $\underline{T}$

Additional Computable Unknowns: r_1, k_1, C_A, C_B, k_2, C_D, $\dot{Q}$

$$k_i = k_{0,i} \exp\left(\frac{-E_i}{RT}\right) \qquad i = 1 \text{ and } 2 \tag{11}$$

$$C_i = \frac{n_i}{V} \qquad i = A, B, \text{ and } D \tag{12}$$

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

IVODE Solver Inputs:

1. Initial values of the reactor model variables shown in Table 1
2. Stopping criterion that n_B equals the final value shown in Table 1
3. Derivatives function that
   a. receives the BSTR model variables (t, n_A, n_B, n_D, n_Z, n_U, and T) at the start of an integration step
   b. returns the corresponding BSTR model derivatives, equations (5) - (10)

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

Variable	Initial Value	Final Value
t	0	t_1
n_A	$n_{A,0} = C_{A,0}V$	
n_B	$n_{B,0} = C_{B,0}V$	$n_{B,f} = 0.01 n_{B,0}$
n_D	0	
n_Z	0	
n_U	0	
T	T_0	

Deliverables Equations:

$$\underline{f}_B = \frac{n_{B,0} - \underline{n}_B}{n_{B,0}} \tag{14}$$

$$\underline{Y}_{D/A} = \frac{\underline{n}_D}{n_{A,0}} \tag{15}$$

$$\underline{\dot{Q}} = UA\left(T_{ex} - \underline{T}\right) \tag{16}$$

$$\underline{\dot{m}}_{H_2O_{(l)}} = \frac{\underline{\dot{Q}}}{\Delta H_{vap}} \tag{17}$$

Implementation of the Calculations

The Python example_7_4_5.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 for a specified conversion of B. The calculations begin by using those functions to solve the design equations for a 99% conversion of B. (Doing so yields corresponding sets of values of the BSTR model variables between 0 and 99%). The results are then used to generate the requested graphs.

Results and Discussion

The calculations were performed as described. The reactions are endothermic, so without heating, the temperature would decrease as they proceed. Here the heating is supplied by the condensation of saturated steam at 220 °F. The initial temperature is 70 °F, and Figure 1 shows that the temperature rises to around 150 °F in the first half hour, and then rises more slowly after that. This is reasonable assuming that the rate is small at 70 °F. In that case, the reaction is not absorbing a significant amount of heat initially. The temperature profile suggests that the rate begins to become significant around 150 °F. From that point on, part of the heat provided by the steam is being consumed by reaction while the rest continues to heat the reacting fluid, so the rate of temperature

increase gets smaller. Figure 2 confirms that the rate begins to become appreciable at ca. 150 °F.

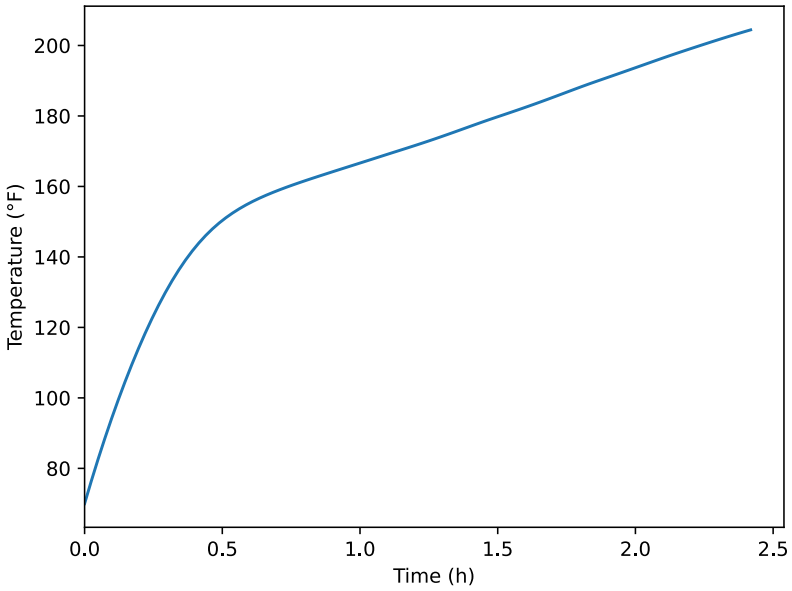

Figure 1. Temperature profile during the process.

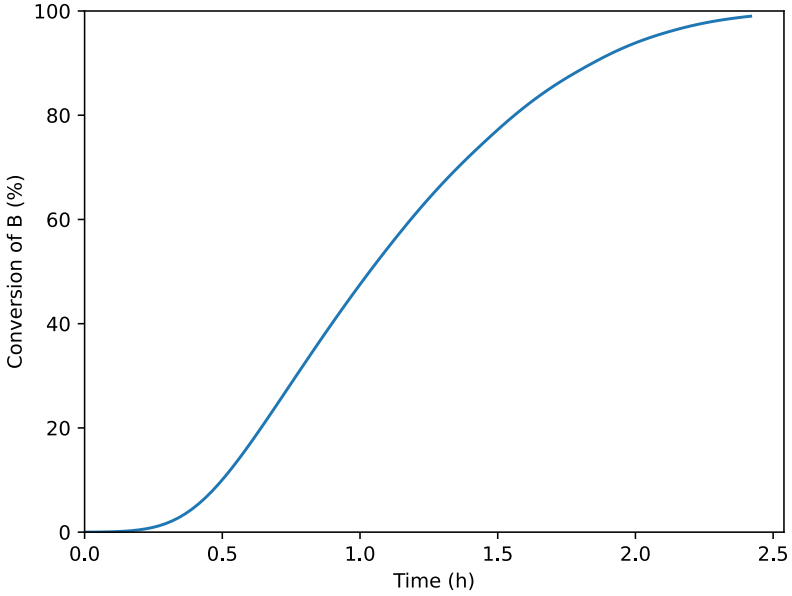

Figure 2. Conversion profile during the process.

The assignment requested a plot of the temperature versus conversion, Figure 3, which can be generated from the results in Figures 1 and 2. The very steep initial rise represents the first half hour during which almost all of the heat provided by the steam was being used to heat the reacting fluid.

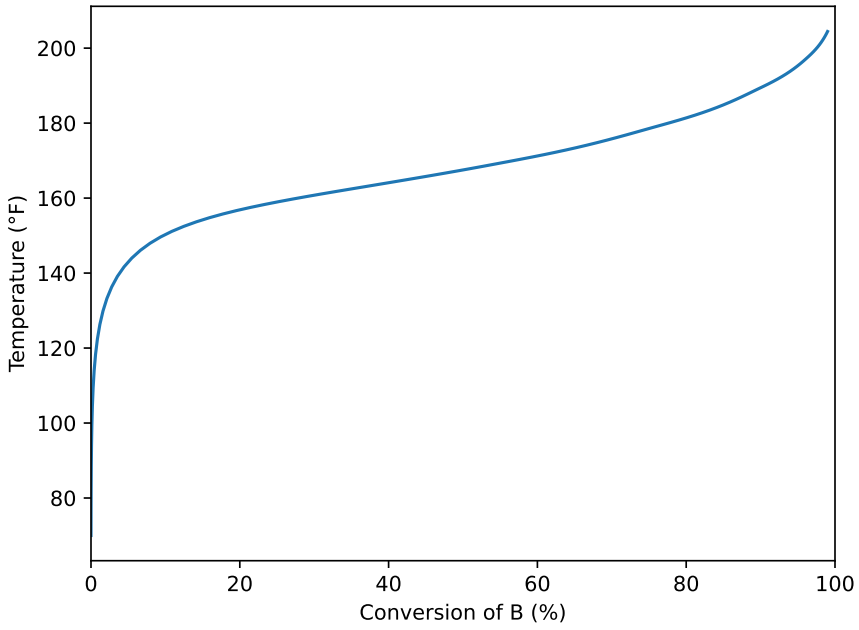

Figure 3. Temperature as a function of conversion.

The steam consumption during the process is shown in Figure 4. Not surprisingly, it mirrors the temperature as a function of conversion. The driving force for heat transfer, and consequently for steam consumption, is the temperature difference between the reacting fluid and the steam. The steam temperature is constant, so changes in the steam consumption track with changes in the reacting fluid temperature. The figures are inverted because as the reacting fluid temperature increases, the temperature difference between it and the steam decreases.

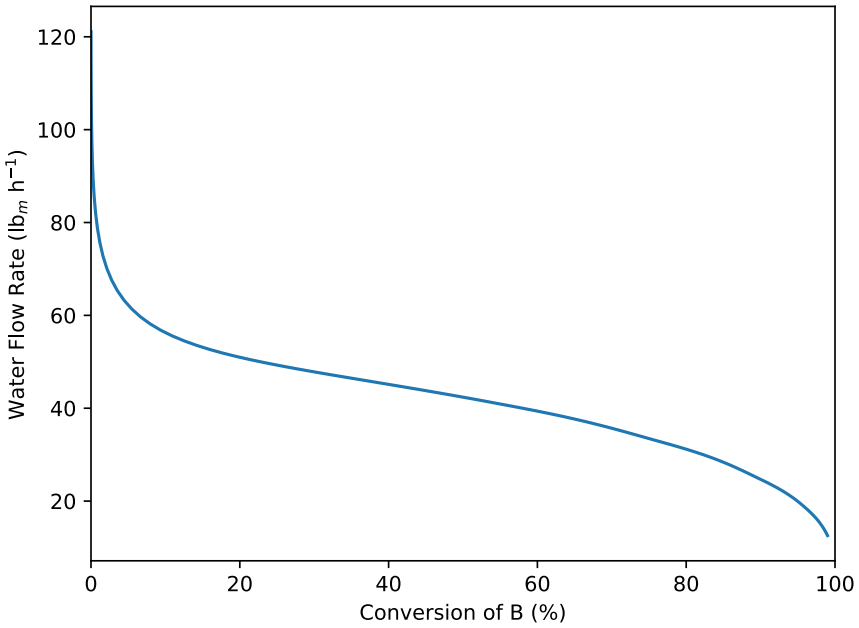

Figure 4. Steam consumption as a function of conversion.

The yield is plotted as a function of the conversion in Figure 5, which shows that it passes through a maximum. This is expected because the reactions are series-parallel reactions, and D is the intermediate product. That is, D is generated by the first reaction and consumed by the second. The reason for the maximum is the same as that provided in Example 5.5.2 of Reaction Engineering Basics. Initially the rate of production of D is large, and due to its small concentration, its rate of consumption is small. As reaction proceeds, the rate of production of D declines due to consumption of the reactants while its consumption increases due to its larger concentration. The concentration of D reaches a maximum when the production and consumption rates become equal. After that, the consumption rate is greater than the production rate and consequently the amount of D decreases.

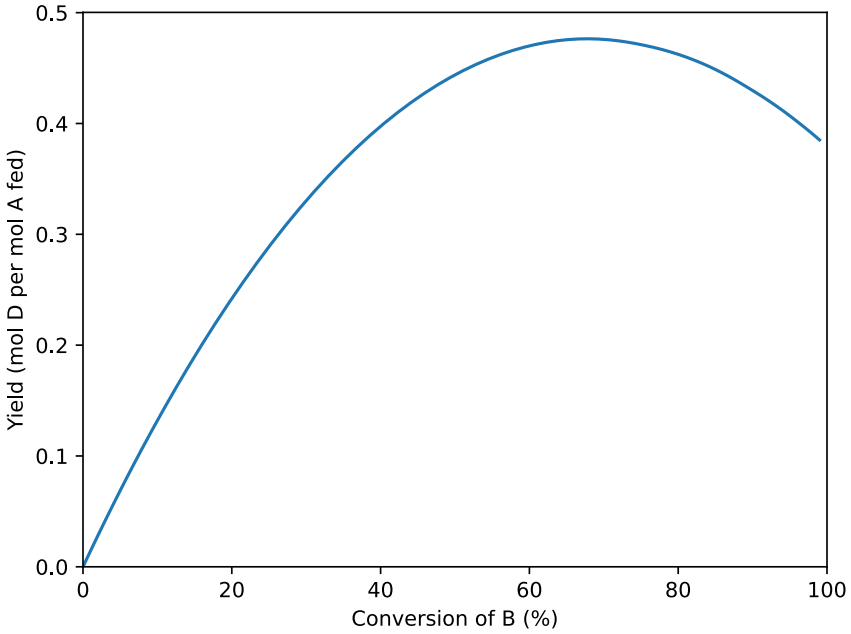

Figure 5. Yield of D from A as a function of reaction progress.

Deliverables

The yield of D from A, temperature, and condensed water flow rates are plotted as functions of the conversion of B in Figures 5, 3, and 4, respectively.