REB, The Course
Class 10 Learning Activity Solution

An ideal, 50 gal CSTR is fed a liquid solution containing 0.014 lbmol A gal^{-1} and 0.020 lbmol B gal^{-1} at a temperature of 70 °F. The heat capacity of the reacting liquid is constant and equal to 65 BTU ft^{-3} °R^{-1}. A jacket surrounding the reactor is supplied with saturated steam at 220 °F. The steam condenses in the jacket, leaving as a saturated liquid. The overall heat transfer coefficient is 60 BTU ft^{-2} °R^{-1} h^{-1}, and the heat transfer area is 13 ft^2. Reactions (1) and (2) take place within the steady-state CSTR. The heat of reaction (1) is 45,000 BTU lbmol^{-1}, and the heat of reaction (2) is 39,500 BTU lbmol^{-1}. The rate expressions for reactions (1) and (2) are given in equations (3) and (4). The rate coefficients 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 54,000 BTU lbmol^{-1}. What volumetric feed rate will maximize the rate of production of reagent D? At that feed rate, what is the conversion of A and the reactor temperature?

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

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

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

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

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, steady-state, non-isothermal CSTR

Given Constants: V = 50 gal, $C_{A,in}$ = 0.014 lbmol gal^{-1}, $C_{B,in}$ = 0.020 lbmol gal^{-1}, T_{in} = 70 °F, $\breve{C}_p$ = 65 BTU ft^{-3} °R^{-1}, T_{ex} = 220 °F, U = 60 BTU ft^{-2} °R^{-1} h^{-1}, A = 13 ft^2, ΔH_1 = 45,000 BTU lbmol^{-1}, ΔH_2 = 39,500 BTU lbmol^{-1}, $k_{0,1}$ = 1.6 × 10^{18} gal lbmol^{-1} h^{-1}, $k_{0,2}$ = 4.5 × 10^{18} gal lbmol^{-1} h^{-1}, E_1 = 46,000 BTU lbmol^{-1}, E_2 = 54,000 BTU lbmol^{-1}.

Parameter: $\dot{V}_{in}$

Deliverables: $\dot{V}_{in,opt} = \underset{\dot{V}_{in}}{\arg\max}\left(\dot{n}_D\right), f_A\Big|_{\dot{V}_{in}=\dot{V}_{in,opt}}$, and $T\Big|_{\dot{V}_{in}=\dot{V}_{in,opt}}$

Formulation of the Equations

Reactor Model Equations:

$$0 = \dot{n}_{A,in} - \dot{n}_A - r_1 V = \epsilon_1 \tag{5}$$

$$0 = \dot{n}_{B,in} - \dot{n}_B - \left(r_1 + r_2\right) V = \epsilon_2 \tag{6}$$

$$0 = -\dot{n}_D + \left(r_1 - r_2\right) V = \epsilon_3 \tag{7}$$

$$0 = -\dot{n}_U + r_2 V = \epsilon_4 \tag{8}$$

$$0 = -\dot{n}_Z + \left(r_1 + r_2\right) V = \epsilon_5 \tag{9}$$

$$0 = \dot{Q} - \dot{V}_{in}\breve{C}_p\left(T - T_{in}\right) - \left(r_1 \Delta H_1 + r_2 \Delta H_2\right) V = \epsilon_6 \tag{10}$$

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

Additional Computable Unknowns: $\dot{n}_{A,in}$, r_1, k_1, C_A, $\dot{V}$, C_B, r_2, k_2, C_D, $\dot{n}_{B,in}$, and $\dot{Q}$

$$\dot{n}_{i,in} = \dot{V}_{in} C_{i,in} \quad i = A \text{ and } B \tag{11}$$

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \tag{12}$$

$$k_2 = k_{0,2} \exp\left(\frac{-E_2}{RT}\right) \tag{13}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \quad i = A, B, \text{ and } D \tag{14}$$

$$\dot{V} = \dot{V}_{in} \tag{15}$$

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

Additional Uncomputable Unknown: $\dot{V}_{in}$

$$\underline{\dot{V}}_{in} = \left[10, \cdots, 100\right] \text{ gal h}^{-1} \tag{17}$$

ATE Solver Inputs:

1. Initial guesses for the reactor model variables

$$\forall \dot{V}_{in,n} \in \underline{\dot{V}}_{in} \qquad \begin{array}{ll} n = 1 & \begin{pmatrix} \dot{n}_{A,guess} = \dot{n}_{A,in} \\ \dot{n}_{B,guess} = \dot{n}_{B,in} \\ \dot{n}_{D,guess} = 0 \\ \dot{n}_{U,guess} = 0 \\ \dot{n}_{Z,guess} = 0 \\ T_{guess} = T_{in} + 5K \end{pmatrix} \\ n > 1 & \begin{pmatrix} \dot{n}_{A,guess} = \dot{n}_A \Big|_{\dot{V}_{in,n-1}} \\ \dot{n}_{B,guess} = \dot{n}_B \Big|_{\dot{V}_{in,n-1}} \\ \dot{n}_{D,guess} = \dot{n}_D \Big|_{\dot{V}_{in,n-1}} \\ \dot{n}_{U,guess} = \dot{n}_U \Big|_{\dot{V}_{in,n-1}} \\ \dot{n}_{Z,guess} = \dot{n}_Z \Big|_{\dot{V}_{in,n-1}} \\ T_{guess} = T \Big|_{\dot{V}_{in,n-1}} \end{pmatrix} \end{array} \tag{18}$$

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

<u>Deliverables Equations</u>:

$$\forall \dot{V}_{in,n} \in \underline{\dot{V}}_{in} \qquad \dot{n}_{D,n} = \dot{n}_D \Big|_{\dot{V}_{in,n}} \tag{19}$$

$$\dot{V}_{in,opt} = \underset{\dot{V}_{in}}{\arg\max} \left(\underline{\dot{n}}_D \right) \tag{20}$$

$$f_A \Big|_{\dot{V}_{in,opt}} = \frac{\dot{n}_{A,in} - \dot{n}_A \Big|_{\dot{V}_{in,opt}}}{\dot{n}_{A,in}} \tag{21}$$

Implementation of the Calculations

The Python script, activity_10.py, that was written to perform the calculations accompanies this solution.

Results and Discussion

The calculations were performed as described above. When the molar flow rate of D was plotted vs. the inlet volumetric flow rate, a maximum was found in the original range of values of $\dot{V}_{in}$ around 45 gal h^{-1}. To improve accuracy, the calculations were repeated using a range from 35 to 50 gal h^{-1}. The results are shown in Figure 1, and the maximum molar flow of D was found to occur at a volumetric feed rate of 44.8 gal h^{-1}.

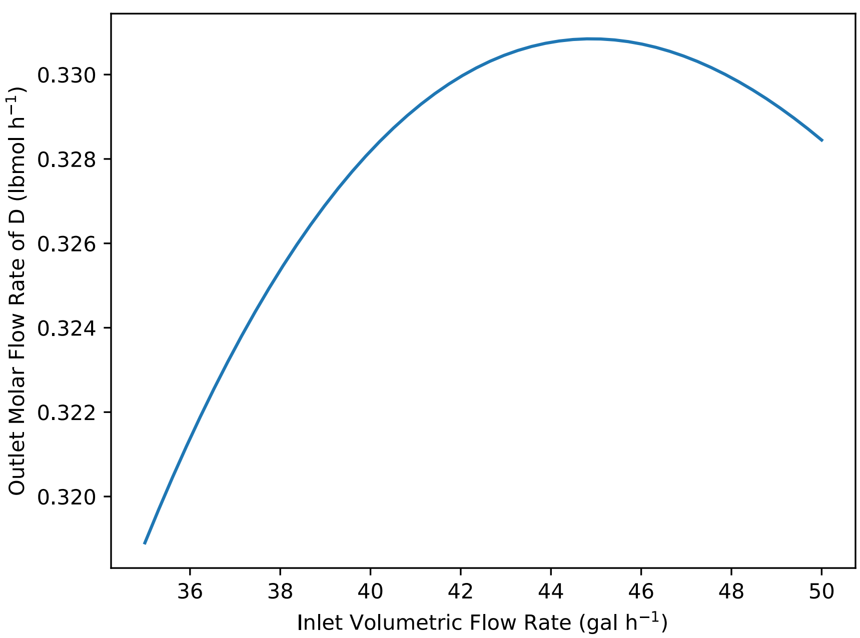

Figure 1. The molar flow of D is maximized at an inlet volumetric flow rate of 44.8 gal h^{-1}.

At the optimum feed rate, the conversion is 52.9% and the outlet temperature is 157 °F. The occurrence of a maximum molar flow rate of D is expected qualitatively (see

Example 5.5.2 in REB, The Book). Reactions (1) and (2) are series-parallel reactions, and D is the intermediate product. At low reaction times (high feed rates), the concentrations of A and B are high leading to a high rate of production of D by reaction (1), and because the concentration of D is small, it's consumption rate is low. As the reaction time increases (feed rate decreases), the rate of generation of D by reaction (1) decreases due to lower concentration of A, while the rate of consumption of D by reaction (2) increases due to higher concentration of D. Eventually, the rate of production of D by reaction (1) decreases to the point where it equals the rate of consumption of D by reaction (2). This is the point where the molar flow of D is maximized. At reaction times higher than this (lower feed rates), the rate of consumption of D is greater than it's rate of generation, so its concentration decreases.

Both reactions are endothermic, but the outlet temperature is significantly greater than the feed temperature. This means that the steam is providing more heat than is being consumed by the reaction. The added heat is likely essential for having a reaction rate that is large enough to get high conversion.

Deliverables

At a feed rate of 44.8 gal min^{-1}, 52.9% of the reactant A is converted. The final temperature is 157 °F.