REB, The Course
Class 9 Practice Assignment Solution

The rate of liquid-phase reaction (1) is adequately described by the rate expression given in equation (2). The rate coefficients exhibits Arrhenius temperature dependence with a forward pre-exponential factor of 1.93 x 10^{13} ft^3 $lbmol^{-1}$ min^{-1}, a reverse pre-exponential factor of 2.86 x 10^{26} min^{-1}, a forward activation energy of 46,400 BTU $lbmol^{-1}$, and a reverse activation energy of 86,700 BTU $lbmol^{-1}$. The heat of reaction (1) is constant and equal to –40,300 BTU $lbmol^{-1}$.

Reactant A is fed to a steady state CSTR at a rate of 0.015 lbmol min^{-1}, and reactant B is fed at a rate of 3.3 lbmol min^{-1}. This corresponds to an inlet volumetric flow rate of 1.41 ft^3 min^{-1}. The CSTR has a fluid volume of 18 ft^3, and it operates adiabatically. The heat capacities of reagent A is 100 BTU $lbmol^{-1}$ $°R^{-1}$, that of B is 18 BTU $lbmol^{-1}$ $°R^{-1}$, and the heat capacity of Z is 120 BTU $lbmol^{-1}$ $°R^{-1}$, and they may be considered to be independent of temperature. What will the conversion and outlet temperatures equal if the combined feed enters at 200 °F.

$$A + B \rightleftarrows Z \tag{1}$$

$$r_1 = k_{1,f} C_A C_B - k_{1,r} C_Z \tag{2}$$

Assignment Summary

<u>Reaction</u>

$$A + B \rightleftarrows Z \tag{1}$$

<u>Rate Expressions</u>

$$r_1 = k_{1,f} C_A C_B - k_{1,r} C_Z \tag{2}$$

<u>Reactor</u>: steady-state, adiabatic, liquid-phase CSTR

<u>Given Constants</u>: $k_{0,f}$ = 1.93 x 10^{13} ft^3 $lbmol^{-1}$ min^{-1}, $k_{0,r}$ = 2.86 x 10^{26} min^{-1}, $E_{1,f}$ = 46,400 BTU $lbmol^{-1}$, $E_{1,r}$ = 86,700 BTU $lbmol^{-1}$, ΔH_1 = -40300 BTU $lbmol^{-1}$, $\dot{n}_{A,in}$ =

0.015 lbmol min^{-1}, $\dot{n}_{B,in}$ = 3.3 lbmol min^{-1}, $\dot{V}_{in}$ = 1.41 ft^3 min^{-1}, V = 18 ft^3, $\hat{C}_{p,A}$ = 100 BTU lbmol^{-1} °R^{-1}, $\hat{C}_{p,B}$ = 18 BTU lbmol^{-1} °R^{-1}, and $\hat{C}_{p,Z}$ = 120 BTU lbmol^{-1} °R^{-1}, and T_{in} = 200 °F.

Deliverables: T and f_A

Formulation of the Equations

Reactor Model Equations:

$$0 = \dot{n}_{A,in} - \dot{n}_A - Vr_1 = \epsilon_1 \tag{3}$$

$$0 = \dot{n}_{B,in} - \dot{n}_B - Vr_1 = \epsilon_2 \tag{4}$$

$$0 = -\dot{n}_Z + Vr_1 = \epsilon_3 \tag{5}$$

$$0 = \left(\dot{n}_{A,in}\hat{C}_{p,A} + \dot{n}_{B,in}\hat{C}_{p,B}\right)\left(T - T_{in}\right) + Vr_1\Delta H_1 \tag{6}$$

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

Additional Computable Unknowns: r_1, k_1, C_A, $\dot{V}$, C_B, C_Z, K_1

$$k_{1,f} = k_{0,f}\exp\left(\frac{-E_{1,f}}{RT}\right) \tag{7}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \qquad i = A, B, \text{ and } Z \tag{8}$$

$$\dot{V} = \dot{V}_{in} \tag{9}$$

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

ATE Solver Inputs:

1. Initial guesses for the reactor model variables

$$\dot{n}_{i,guess} = \dot{n}_{i,in} \qquad i = A, B, \text{ and } Z \tag{11}$$

$$T_{guess} = T_{in} + 5K \tag{12}$$

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

Deliverables Equations:

$$f_A = \frac{\dot{n}_{A,in} - \dot{n}_A}{\dot{n}_{A,in}} \tag{13}$$

Implementation of the Calculations

The Python practice_9.py, that was written to perform the calculations accompanies this solution. It defines a CSTR model function and a CSTR residuals function that solve the design equations by calling an ATE solver. The results are used to calculate the final conversion.

Results and Discussion

The calculations were performed as indicated above. The outlet temperature is 227 °F and the conversion is 33.4%. The 27 °F temperature rise is consistent with the reaction being exothermic and the reactor operating adiabatically. The heat released by the reaction is not removed, so the temperature increases.

Even though there is a huge excess of reagent B, the conversion of reagent A is not that large. This indicates that the reverse reaction is significant at reaction conditions. If that is true, increasing the temperature will not increase the conversion, and may even decrease it because for an exothermic reaction, the conversion decreases as the temperature increases. Another way of putting that is that for an exothermic reaction, the rate of the reverse reaction increases faster with temperature than the rate of the forward reaction.

Deliverables

When the feed to the CSTR is at 200 °F, the outlet temperature is 227 °F and the conversion is 33.4%..