PFR with inter stage cooling: Example 8.6, with some modifications

Consider the following liquid phase elementary reaction: \( A \rightleftharpoons B \). It is an exothermic reaction with \( \Delta H = -20 \text{ kcal/mol} \). The feed is pure A, at 300 K. The specific heat capacities are \( C_{p,A} = C_{p,B} = 50 \text{ cal/mol/K} \).

1. Plot equilibrium conversion \( X_e \) vs Temperature
2. Plot the maximum possible conversion if it is operated adiabatically.
3. Assume that we have three reactors of sufficient volume that for any feed temperature, we can achieve 95% of \( X_e \) and that the reactors are operated adiabatically. We have coolant coming in at 270 K and can’t be heated beyond 400 K. The coolant \( C_p \) is 18 cal/mol/K. We can use these to cool the out coming fluid to 350 K. What is the maximum conversion achievable? What is the load on the heat exchanger? Assume that \( U = 100 \text{ cal m}^{-2} \text{ K}^{-1} \text{s}^{-1} \) and that the feed is 40 mol/s
4. Data: We have one PFR, which has to be operated adiabatically. The feed comes at 40 mol/s and the volumetric flow rate is 10 lit/s. The rate constants are \( k_1 = 4.5 \times 10^4 e^{1.987T} \text{ s}^{-1} \) and \( k_{-1} = 2.1 \times 10^{11} e^{1.987T} \text{ s}^{-1} \). (This would match the data given in the book to a reasonable extent). Find the optimal inlet temperature, if the PFR volume is 100 lit, if the PFR volume is 500 lit etc.

Solution:
1. We actually use the \( k_1 \) and \( k_{-1} \) value given and calculate the equilibrium constant and then the conversion as a function of temperature. The results are shown below.

![Equilibrium Conversion vs Temperature](image)

2. If operated adiabatically, with \( T_{in} = 300 \text{ K} \), we have the following heat balance equation.
\[
F_{A-in} \Delta H = \sum_i F_{i-in} C_{p-i} (T - T_{in})
\]
This is because the specific heat capacities and heat of reaction are independent of temperature.
Since we send pure A, this equation reduces to
The outlet temperature will be 460 K, and the equilibrium conversion will be 0.40 (roughly). This is slightly different from the problem described in the book because the equilibrium constant value is slightly different.

3. Inter stage cooling.

First Reactor:
At the outlet of the first reactor, the conversion = 95% of X_e = 0.95 * 0.4 = 0.38. At that conversion, the temperature is 452 (since T = 300+400x)

This is at 460 K. It must be cooled to 350 K. The heat removed = \( F_A C_{p-A} + F_B C_{p-B} \) \((452–350) = 40\times50\times102 = 204,000 = 204\text{kcal/s} \)
Since \( C_{p-A} = C_{p-B} \), this calculation is simple.

Second Reactor:
Now, the \( F_{A-in} \) for the second reactor is \( F_{A-out} \) of the first reactor. \( F_{A-in} (1 – x) = 40(1–0.38) = 24.8 \text{mol/s} \) and the \( F_{B-in} \) for the second reactor is 15.2 \text{mol/s} \). This comes at 350 K (because we have cooled this stream).
With this feed, the equilibrium conversion is calculated as follows. The $X_e$ vs Temperature curve remains the same. But the heat balance equation will be

$$F_{A,in} x (-\Delta H) = \left( \sum F_{i,\text{in}} C_{p,i} \right) (T - T_i)$$

and in this case

$$40 \times (x - 0.38) (20000) = 40 \times 50 \times (T - 350)$$

This is simplified as

$$x = 0.38 + \frac{50}{20000} \times (T - 350)$$

This meets the equilibrium conversion line at 443 K and 0.6125 conversion. 95% of that is 0.5819. In the energy balance line, the temperature corresponding to that is 431 K. This is to be cooled to 350 K.

The load on the second heat exchanger will be $40 \times 50 \times (431 - 350) = 162 \text{kcal/s}$

**Third Reactor:**

The energy balance equation for the third reactor is

$$40 \times (x - 0.5819) (20000) = 40 \times 50 \times (T - 350)$$

The equilibrium conversion is 0.776 and the temperature at the outlet will be 428. But we get 95% of the equilibrium conversion, i.e. 0.7372 and the corresponding temperature is 412 K.

**Heat Exchanger load:**
The overall cooling load is $204 + 162 \text{ kW} = 366 \text{ kW}$

The load on the first heat exchanger: $F_c C_p (400 - 270) = 204 \text{ kW}$, implies flow rate needed is 87.2 mol/s.

The load on the second heat exchanger is about 69 kg.

The area needed is calculated assuming counter current heat exchanger.

$$LMTD = \frac{(452 - 400) - (350 - 270)}{\ln \left( \frac{452 - 400}{350 - 270} \right)} = 65 \text{ K}$$

Given $U = 100 \text{ W/m}^2\text{K}$, we get $U \times A \times LMTD = 204 \text{ kW}$
Therefore the area of the heat exchanger must be 31.4 m$^2$.

For the second heat exchanger,

$$LMTD = \frac{(431 - 400) - (350 - 270)}{\ln \left( \frac{431 - 400}{350 - 270} \right)} = 51.7 \text{ K}$$

Therefore, the heat exchanger area must be also 31.4 m$^2$. The heat load is less, but the LMTD is also less.

**Volume of the reactors 1, 2 and 3.**

As an extra, we will also calculate the volume of the reactor needed at each stage.

The mass balance equation is

$$\frac{dV}{dx} = \frac{Q}{k_1 (1-x) - k_2 x}$$

The heat balance equation is

$$F_{A-in} (x-x_{in}) (-\Delta H) = \left( \sum_i F_{i-in} C_{p-A} \right) (T - T_{in})$$

i.e. $T = T_{in} + \left( x - x_{in} \right) \frac{(-\Delta H)}{C_{p-A}}$

For the first reactor, $T_{in} = 300 \text{ K}, x_{in} = 0, x_{out} = 0.38$.
For the second reactor, $T_{in} = 350 \text{ K}, x_{in} = 0.38, x_{out} = 0.5819$.
For the third reactor, $T_{in} = 350 \text{ K}, x_{in} = 0.5819, x_{out} = 0.7372$. 

First Reactor volume is 1215 lit
Second Reactor volume is 623 lit
Third Reactor volume is 803 lit

4. Vary $T_{in}$ and find the outlet conversion

The design equation is

$$\frac{dF_A}{dV} = -k_1C_A + k_2C_B$$

Since the feed contains pure A and since it is in liquid phase, we can write

$$F_{A-in} \frac{dx}{dV} = k_1C_{A-in} (1-x) - k_2C_{A-in}x$$

This can be simplified as

$$\frac{dx}{dV} = \frac{k_1(1-x) - k_2x}{Q}$$

The heat balance equation is of course given by

$$F_{A-in} x (-\Delta H) = F_{A-in} C_{p-A} (T - T_{in})$$

which can be written as

$$T = T_{in} + \frac{(-\Delta H)}{C_{p-A}}x$$
For the values given, the ‘best’ temperature at the inlet is 427 K, and we can achieve a conversion of about 13.5%. If the volume of the PFR is 500 lit, then best inlet temperature is 347 K with a corresponding conversion of 30%.

If the PFR volume is 1000 lit, then best $T_{in}$ is 312 K and the conversion is about 37%. If the PFR volume is 2000 lit, the best $T_{in}$ is 282 K and the conversion is 43.7%.

As the volume of the reactor increases, the conversion comes close to the equilibrium conversion; Also, any variation in the inlet temperature causes a steep loss in the conversion, i.e. the conversion becomes very sensitive to inlet temperature, especially at the ‘cooler’ side.

**Final:** We know that for one reactor, under adiabatic operation, we can get at the most 40% (slightly higher than that) conversion. What do we get if we ask the program to find the volume to get 50% conversion?

We get a warning that it is not able to integrate beyond 40%.

“Warning: Failure at t=4.009973e-001. Unable to meet integration.
tolerances without reducing the step size below the smallest value allowed (8.881784e-016) at time t.

> In ode45 at 371
  In PFRInterstage at 188

We get that for a PFR volume of 1342.0644 lit, a conversion of 40% is possible. Beyond that, we can’t get any result.