6.7: ODE and Excel Model of an Adiabatic PFR

7.1 Introduction

A plug flow reactor (PFR) is a tubular reactor used in chemical reactions. Reactants enter one end of the PFR, while products exit from the other end of the tube. A PFR is useful because of high volumetric conversion and good heat transfer. PFRs carry out power law reactions faster than CSTRs and generally require less volume. Excel modeling for an adiabatic plug flow reactor is useful for estimating conversion as a function of volume. By inputting the values of the constants and iteratively changing the volume, the conversion at a specific volume can be determined. This removes the need for complicated hand calculations and helps the user visualize the reaction and notice trends through the PFR. Alternatively, excel modeling can also determine the temperature inside the reactor as a function of volume. Euler's integration is used to estimate the conversion or temperature through the PFR. By ensuring that the volume intervals are small, the conversion or temperature values generated should be fairly accurate. Refer to the Euler's method section for more information on its implementation.
7.2 Basic Algorithm to Model Adiabatic PFR

The model presented will include the following assumptions:

1. Negligible pressure drop
2. Single elementary reaction
3. Power law kinetics
4. Constant fluid properties (i.e. heat capacity)

To describe the basic algorithm for an adiabatic PFR, a simple case will be considered where pure A enters the reactor:

\[ \ce{aA <=> aB} \]

1. Reactor Type

PFR

2. Limiting Reagent

The design and rate equations should be expressed in terms of the limiting reagent. Here, A is the limiting reagent.

3. Design Equation

The design equation for a PFR can be expressed in terms of several variables, including conversion, moles, and concentration. It is important to note that the design equation in terms of conversion may only be used if one reaction is occurring. Otherwise, it must be expressed in terms of moles or concentration. The equation to describe conversion as a function of volume, as derived from a simple mole balance, is shown below in Equation 1.

\[
\frac{d X}{d V} = \frac{-r_A}{F_{AO}} \tag{1}
\]

- \(X\) = conversion
- \(V\) = volume
- \(r_A\) = reaction rate of A
- \(F_{AO}\) = initial moles of A
4. Rate Law

The rate law is independent of reactor type. It is expressed in terms of a rate constant and concentration. If the reaction is irreversible, the rate law is modeled according to Equation 2. If the reaction is reversible, the rate law models Equation 3 in which the concentration of B and the equilibrium constant must be accounted for.

\[
\begin{align}
-r_{A} &= k c_{A}^{a} \quad \text{\label{2}} \\
-r_{A} &= k\left(c_{A}^{a}\right)-\frac{c_{B}^{b}}{K_{C}} \quad \text{\label{3}}
\end{align}
\]

where

- \(k\) = rate constant
- \(c_{A}^{a}\) = concentration of \(A\) with stoichiometric coefficient \(a\)
- \(c_{B}^{b}\) = concentration of \(B\) with stoichiometric coefficient \(b\)
- \(K_{C}\) = equilibrium constant

If the reaction is not isothermal, the rate constant and equilibrium constant should be written in terms of temperature as shown in Equation 4 and 5.

\[
\begin{align}
k &= k_{0} \exp \left(\frac{E}{R}\left(\frac{1}{T_{0}}-\frac{1}{T}\right)\right) \quad \text{\label{4}} \\
K_{C} &= K_{C 1} \exp \left(\frac{\Delta H_{RX}}{R}\left(\frac{1}{T_{1}}-\frac{1}{T}\right)\right) \quad \text{\label{5}}
\end{align}
\]

where

- \(k_{0}\) = rate constant at \(T_{0}\)
- \(E\) = activation energy
- \(R\) = ideal gas constant
- \(T\) = temperature
- \(K_{C 1}\) = equilibrium constant at \(T_{1}\)
- \(\Delta H_{RX}\) = standard heat of reaction

5. Stoichiometry

Stoichiometry is used to express concentration of a species in terms of concentration of the limiting reactant. The stoichiometry equation depends on whether the reaction occurs in the liquid or gas phase. If it occurs in the gas phase, Equations 6 and 7 are used. For liquid phase, \(\epsilon\) becomes zero and the correlation reduces to Equation 8. There is no pressure term included because it is assumed that pressure drop is negligible, and the initial pressure is equal to the final pressure.

\[
\begin{align}
C_{A} &= C_{A o} \cdot \frac{(1-X)}{(1+\epsilon \cdot X)} \cdot \frac{T_{0}}{T} \quad \text{\label{6}} \\
\end{align}
\]

\[
\begin{align}
K_{c} &= K_{c 1} \cdot \frac{\Delta H_{RX}}{R} \cdot \frac{T_{0}}{T} \quad \text{\label{7}}
\end{align}
\]

where

- \(k_{0}\) = rate constant at \(T_{0}\)
- \(\epsilon\) = activity energy
- \(R\) = ideal gas constant
- \(T\) = temperature
- \(K_{C 1}\) = equilibrium constant at \(T_{1}\)
- \(\Delta H_{RX}\) = standard heat of reaction
\[ \frac{C_{B}}{C_{A}} = C_{A_0} \frac{\left(\theta_{B} + \frac{b}{a} x\right)}{1 + \epsilon x} \frac{T_0}{T} \] \quad (7)

\[ C_{A} = C_{A_0} (1 - x) \] \quad (8)

\[ C_{B} = C_{A_0} \left(\theta_{B} + \frac{b}{a} x\right) \] \quad (9)

where

- \( \epsilon = y_{A_0} \) (stoichiometric coefficients of products - coefficients of reactants)
- \( y_{A_0} \) = initial mole fraction of A
- \( \theta_i \) = ratio of initial moles (or concentration) of species \( i \) to initial moles (or concentration) of A

6. Combine

The design equation, rate law, and stoichiometric equations are combined. For example, assume the reaction is irreversible, liquid phase, and isothermal, with pure A entering the reactor and has the combined equation as shown below.

\[ \frac{d X}{d V} = \frac{k \cdot C_{A_0}^a (1 - x)^a}{F_{A_0}} \] \quad (10)

7. Energy Balance

The energy balance can be used to relate temperature and conversion. It assumes heat flow and shaft work are not present.

\[ T = \frac{X \left(-\Delta H_{RX}\right) + \sum \Theta_i C_{p_i} T_0 + X \Delta C_{p} T_r}{\sum \Theta_i C_{p_i} + X \Delta C_{p}} \] \quad (11)

with

- \( C_{p_i} \) = heat capacity of species \( i \)
- \( \Delta C_p \) = \( C_p \) products- \( C_p \) reactants

If \( \Delta C_p = 0 \), the energy balances reduces to the following:

\[ T = \frac{X \left(-\Delta H_{RX}\right) + \sum \Theta_i C_{p_i} T_0}{\sum \Theta_i C_{p_i}} \] \quad (12)

8. Solve

Solve the system of equations in Excel. The ODE is approximated by Euler's method. See the attached spreadsheet for the ODE/Excel modeling of the adiabatic PFR.

7.3 Using The Excel Model

On the "Reaction Scheme" worksheet enter the various stoichiometric values for your reaction, the specific heats for the various reactants and products, and also the heat of reaction and the reference temperature that the heat of reaction is
The "Input Conditions" worksheet is fairly straightforward. If the reaction is gas-phase make sure to enter a "1" in the appropriate cell and if liquid-phase enter a "0".

The "Rate Law" sheet contains the definitions for the values you will have to enter on this sheet. Note that T1 is the reference temperature for your rate constant. Make sure to enter a "1" in the cell if your reaction is reversible, and a "0" if it is irreversible.

Make sure not to tamper with the "Numerical Calculations" worksheet! You can, however, scroll downward to extract exact values for volume, conversion, and temperature down the PFR.

Multiple reactions are not included in this model. Having multiple reactions would require a separate reaction scheme sheet for every reaction, and would require many different adjustments to ensure that all scenarios are accounted for.

Example \(\PageIndex{1}\)

A plant at the ETF (Equipment Testing Facility) has been acquired in a hostile takeover by Brown Industries, a company for which you are a process engineer. The Engineering Manager, Phil Savage, has assigned you to work on a PFR located within this new plant. The particular PFR in question is used to conduct the following reaction:

\[
\ce{A \rightarrow B}
\]

He wants you to provide him with two pieces of information. First, he wishes to know how far down the reactor must the reaction go to achieve 80% conversion. Secondly, he wants to know the temperature at this point.

You decide that first it would be best to ascertain all the thermodynamic and kinetic properties that are inherent to this reaction. Instead of looking them up in Perry's or your old ChemE books, however, you decide to ask the Lead Plant Engineer, Pablo LaValle. Pablo tells you the following:

"Listen wisely to what I say, young grasshopper. This reaction is irreversible, liquid-phase, and elementary. We will feed the reactants into the tube reactor of diameter 50cm at 273 K. We will begin with an initial concentration of A at 1.6 mol/L and an initial molar flow rate of A at 2 mol/min. The heat of reaction at 300 K is -20 kJ/mol A. The rate constant at 300K is 0.2 mol / L * min. The activation energy at 300K is 15.2 kJ/mol. The Cp values for the products and reactants are as follows.

- Cp A = 200 J / mol K
- Cp B = 100 J / mol K

"Go forth and use the Excel sheet that Group B has created and your job will be very easy."

**Solution**

The model for this example can be found here.

Pablo gave all the data needed to complete the model. After inputting the data, the final page of the spreadsheet was used to determine the reactor conditions Savage desired.
X = 0.8 at a reactor length of 33.4 meters. The temperature at this point of the reactor is 388.4K.

Example \ref{PageIndex2}

You have just completed your initiation in the ultra-super secret elite society known as the League of Chemical Engineers which is headquartered high in the Himalayans. They have an adiabatic PFR (diameter = 10cm) in their possession which they use to produce two gases, known as B and C, from a gas-phase reactant known as A. The reversible gas reaction is shown below:

\[
\ce{ A <=-> B + C}
\]

Your sensei wishes to know what the maximum conversion possible is and also what length of reactor would be needed to reach a conversion of 15%. First, however, he orders you to climb K2 where the reaction data is stored by the society. After a perilous 5 day journey you discover the following information:

- \(C_p \ A = 40 \text{ kJ/mol K}\)
- \(C_p \ B = 25 \text{ kJ/mol K}\)
- \(C_p \ C = 15 \text{ kJ/mol K}\)
- \(C_{AO} = 0.271 \text{ mol/L}\)
- \(F_{AO} = 5 \text{ mol/min}\)
- Initial Temp = 450K
- Heat of reaction at 300K = -20 \text{ kJ/mol A}
- Activation energy = 31.4 \text{ kJ/mol}
- \(K_{eq} \text{ at 300K} = 0.01 \text{ mol/L}\)
- \(k_{\text{forward}} \text{ at 300K} = 0.133 \text{ mol/(L*min)}\)

Solution

After climbing back down K2, and finding a computer, the data obtained can be input into the adiabatic model. The solution can be found here.

Be sure to set the values for both gas phase reaction and reversible reaction to 1.

Using the data table found on the last page of the spreadsheet, the desired information can be extracted.

The maximum conversion that can be achieved is \(X = 0.187\)

The reactor requires 64.8 meters to achieve a conversion of 15%.

References

Contributors and Attributions

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