Design of a Plug Flow Reactor (PFR)

**Problem definition**

The following reactor design problem was taken from Fogler [1] page 149 Example 4-4:

Determine the plug flow reactor volume necessary for the production of 300 $10^6$ lbmol/year of ethylene from ethane pyrolysis. Assume an irreversible reaction that follows an elementary first order rate law. It is desired to achieve 80% conversion of ethane, operating the reactor isothermally at 1100 K and a pressure of 6 atm.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rate constant $k$ at $T=1000$ K</td>
<td>0,072 s$^{-1}$</td>
</tr>
<tr>
<td>Rate constant $k$ at $T=1100$ K</td>
<td>3,07 s$^{-1}$</td>
</tr>
<tr>
<td>Reaction temperature $T$</td>
<td>1100 K</td>
</tr>
<tr>
<td>Reaction pressure $P$</td>
<td>6 atm</td>
</tr>
<tr>
<td>Conversion of Ethane $X_{C2H6}$</td>
<td>0,80</td>
</tr>
<tr>
<td>Molar flow rate of Ethylene $F_{C2H4}$</td>
<td>$300 \times 10^6$ lbmol/year</td>
</tr>
</tbody>
</table>

**Solution principle**

CHEMCAD allows you with the kinetic reactor model to evaluate a plug flow reactor (PFR) or a continuous stirred tank reactor (CSTR). Both reactors have two operation modes: rating or design mode. In the first one, it is possible to calculate the conversion if the user specify the volume and the second one permits you to calculate the required volume of the reactor knowing the desired conversion of a key component.
Figure 1 shows the setup of the flow sheet in CHEMCAD.

The PFR model is a rigorous model, which can simulate tubular reactors. The basic assumptions of this model are that no axial mixing or heat transfer occurs (Plug Flow). The CHEMCAD kinetic reactor unit has five operation modes: Isothermal, adiabatic, specified heat duty, specified temperature profile and specified utility conditions. Its utilities may be co-current or counter-current. The simulation of this type of reactor requires a general definition of the reactor, the stoichiometry and rate data for each reaction. Up to 20 simultaneous reactions can be defined.

The reaction that takes place in this reactor is the ethane dehydrogenation. Consequently, ethylene and hydrogen are obtained, all in gas phase (g):

\[ \text{C}_2\text{H}_6 (g) \rightarrow \text{C}_2\text{H}_4 (g) + \text{H}_2 (g) \]

Based on the information given by Fogler this is an irreversible first order reaction, which leads to the rate equation (1)

\[ -r_{C_2H_6} = k \cdot C_{C_2H_6} \]
Where:

$C_{C_2H_6}$: concentration of ethane

$-r_{C_2H_6}$: reaction rate of ethane

$k$: rate constant

The rate constant $k$ is temperature dependent. It temperature dependency can be calculated with the Arrhenius approach, see equation (2).

$$k = A \cdot e^{-\frac{E_a}{RT}}$$

(2)

Where:

$k$: kinetic constant

$A$: frequency factor

$E_a$: activation energy

$R$: gas constant (1,987 cal/molK = 8,314 J/molK)

$T$: absolute temperature

The frequency factor and the activation energy can be determined graphically as shown in figure 2.

![Graphical determination of kinetic parameter](image)

Figure 2. Graphical determination of kinetic parameter

The resulting values are $A = 6.04 \times 10^{16} \text{1/s}$ and $E_a = 82 \text{kcal/mol}$. 
Assuming 80% of conversion of the Ethane the required feed stream can be calculated with the following equation:

\[
F_{C_2H_6} = \frac{300 \times 10^6 \text{lb ethylene}}{\text{year}} \times \frac{453.6 \text{ g ethylene}}{28 \text{ g ethylene}} \times \frac{\text{mol ethylene}}{\text{year}} \times \frac{1}{365 \text{ day}} \times \frac{1}{24 \text{ h}} \times \frac{1}{3600 \text{ s}} \times \frac{0.8 \text{ mol ethylene}}{\text{mol ethane}} = 192,64 \text{ mol ethane / s}
\]

**Implementation of the kinetic reactor in CHEMCAD**

The simulation is performed with CHEMCAD Steady State. Prior to the simulation, the components and the thermodynamic model must be selected. At “Thermophysical: Select components”, the components ethane (CAS no.: 74-84-0), ethylene (CAS no.: 67-64-1) and hydrogen (CAS no.: 110-05-4) are selected. The subsequent "Thermodynamics Wizard" suggests a suitable model after specification of the pressure and the temperature. For the given example, CHEMCAD suggests the k-value model and the enthalpy model, SRK. Furthermore, at “Format: Engineering Units”, metric units are selected and pressure units changed to “atm”, time units to “seconds”, temperature units to “Kelvin” and mass/mole units to “mol”.

The UnitOp (unit operation) for the kinetic reactor is entered in the flow sheet and a feed and a product stream are allocated. The feed stream is set with the data stated in table 2 (see figure 3).

**Table 2: Relevant data for the example simulation**

<table>
<thead>
<tr>
<th>Units</th>
<th>Components</th>
<th>Thermodynamics</th>
<th>Feed streams</th>
<th>Unit operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metric (modified)</td>
<td>Ethane, Ethylene,</td>
<td>K: SRK, H: SRK</td>
<td>( T = 1100 \text{ K} )( p = 6 \text{ atm} ) ( F_{C_2H_6} = 192,64 \text{ mol / s} )</td>
<td>1 kinetic reactor (KREA) 1 feed 1 product</td>
</tr>
<tr>
<td></td>
<td>Hydrogen</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The kinetic reactor is initialized in the next step. In the settings window (figure 4), two different design options at "Reactor Mode" can be selected. For this case, we will select PFR (plug flow reactor). The following inputs are required to initialize the PFR: number of reactions, thermal mode, calculation mode, reactor pressure, pressure drop and temperature, reaction phase and kinetic rate expression.

In this example, we only have one reaction and the reactor is operated at 1100 K so the isothermal mode is selected. As both streams are gases, the “vapor only” option is selected. Now the Calculation mode and the kinetic rate expression have to be defined. The conversion of key component is the design parameter, so that the options “Specify conversion, Calculate volume” and “Standard-all reactions” are selected respectively (see figure 4).

In the second tab of the KREA screen (More specifications) the reaction engineering units of the rate law must be adjusted according to the units of $A$ and $E_a$ as defined earlier, see figure 5.
After pushing the OK button a new window appears and the rate law parameters, the stoichiometric coefficients, and exponential factor can be entered, as shown in figure 6.

Figure 5: "More specifications" settings window

Figure 6: "Kinetic data" settings window
The simulation is now ready to run.

Assessment of the simulation results

In order to obtain a simple overview of the process, the calculated reactor properties and the stream characteristics can be shown in the flow sheet by using “Format - Add stream box”/ “Format - Add UnitOp box”, see figure 7.

![Figure 7: Results after the simulation of the PFR.](image)

We can see that the requested Ethane conversion and the outlet mole rate of ethylene are achieved. A PFR volume of 2.28 m³ is needed for the dehydrogenation of 192.64 mol/s of ethane. This calculated reactor volume is in accordance with the result given by Fogler.

For further analysis different profiles through the reactor can be plotted. These can be selected at “Plot - UnitOp Plots”/ “Plug flow reactor profile”, see figure 8.
Approaches for the optimization of plug flow reactors

The parameters of the reactor can be analysed and optimised easily with CHEMCAD. This can be done with a sensitivity study, which can be configured at “Run-Sensitivity study” / “New Analysis”.

Figure 9 shows the influence of the reaction pressure on the required reactor volume under the given conditions, while figure 10 shows the impact of a varying reactor temperature.
Figure 9: Required reactor volume with pressure change.

Figure 10: Required reactor volume with temperature change.
The above simulation was generated in CHEMCAD 6.5.3
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Sources: