Homework 3 – Ammonia Reactor Design

Ammonia (NH₃) is produced by the Haber-Bosch process. In designing an efficient process for Ammonia, the single pass reactor conversion should be maximized with as small a capital cost as possible. Using “Engineering Tricks” discussed in Lecture 6, develop an Aspen Simulation for such a reactor maximizing the conversion.

The Haber-Bosch ammonia synthesis reaction is written as:

\[ 0.5 \text{N}_2 + 1.5 \text{H}_2 \leftrightarrow \text{NH}_3 \]

using an iron on Al₂O₃ catalyst with a particle density of 3 gm/mL, particle size of 2 mm and a void fraction of 0.6. A process schematic of the Haber-Bosch process is given in Figure 1.

Thermodynamic Data for this reaction is given in Table 1. With some calculations, this data suggests that the ammonia synthesis reaction is exothermic and spontaneous, i.e. \( \Delta G_{\text{rxn}} \) is negative.

Table 1 Thermodynamic Data at 298.15°K (25°C). Data from Ring, T.A. Fundamentals of Ceramic Powder Processing and Synthesis,” Academic Press, 1996.

<table>
<thead>
<tr>
<th></th>
<th>( \Delta H^\circ ) [kcal/mol]</th>
<th>( \Delta G^\circ ) [kcal/mol]</th>
<th>S°[cal/deg/mol]</th>
<th>C°p[cal/deg/mol]</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂(g)</td>
<td>0</td>
<td>0</td>
<td>31.208</td>
<td>6.889</td>
</tr>
<tr>
<td>N₂(g)</td>
<td>0</td>
<td>0</td>
<td>45.77</td>
<td>6.961</td>
</tr>
<tr>
<td>NH₃(g)</td>
<td>-11.02</td>
<td>-3.94</td>
<td>45.97</td>
<td>8.38</td>
</tr>
<tr>
<td>CH₄(g)</td>
<td>-17.88</td>
<td>-12.13</td>
<td>44.492</td>
<td>8.439</td>
</tr>
<tr>
<td>Ar(g)</td>
<td>0</td>
<td>0</td>
<td>36.9822</td>
<td>4.9679</td>
</tr>
</tbody>
</table>

The reactor feed for this world class plant comes from two sources: 1) fresh feed and 2) recycle. These two feed streams to the reactor have the following characteristics:

<table>
<thead>
<tr>
<th></th>
<th>Fresh Feed Flow Rate 20,000 kmol/hr</th>
<th>Recycle 40,000 kmol/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>25°C and 150 atm</td>
<td>Mole %</td>
<td>Mole %</td>
</tr>
<tr>
<td>H₂</td>
<td>72</td>
<td>61</td>
</tr>
<tr>
<td>N₂</td>
<td>24</td>
<td>20</td>
</tr>
<tr>
<td>NH₃</td>
<td>0</td>
<td>1.5</td>
</tr>
<tr>
<td>CH₄</td>
<td>3</td>
<td>13</td>
</tr>
<tr>
<td>Ar</td>
<td>1</td>
<td>4.5</td>
</tr>
</tbody>
</table>
Fresh feed is produced from two sources one for the hydrogen primarily and the other for the nitrogen primarily:

1) Syngas produced by the partial combustion of methane, water gas shift reaction with the removal of CO₂ via amine adsorption and then CO via methanation¹ and

2) Nitrogen from an air separation plant.

The impurity CH₄ comes from the syngas process and the impurity Ar comes from Air used in both the syngas process and the air separation plant. Both of these impurities decrease the partial pressure of the reactants and as a result lower the reaction rate given by²:

\[
\text{Rate}_{\text{N}_2} = 10^4 \text{kmol/}(m^3s) \exp(-91 \text{kJ/mol}/(R_gT)) \left[P_{\text{N}_2}/\text{atm}\right]^{0.5} \left[P_{\text{H}_2}/\text{atm}\right]^{1.5} \\
- 1.3 \times 10^{10} \text{kmol/}(m^3s)\exp(-140 \text{kJ/mol}/(R_gT)) \left[P_{\text{NH}_3}/\text{atm}\right]
\]

Please note that the reaction has both forward and reverse rates indicating that the reaction will go to equilibrium for a very long catalytic reactor.

To limit the range of variables considered in your reactor design, please use one to a maximum of three catalytic Shell and Tube-type reactors that each are up to 20 ft long and have up to 1000 tubes in the shell. The tubes which are loaded with catalyst cannot be larger than 2 inches in diameter to dissipate heat from the catalyst. Tubes are typically not smaller than 2 inch in diameter to allow for ease of filling the tubes with catalyst particles. The catalyst cost is $ 30/kg. As a result of the exothermic reaction and high pressure materials of construction need to be considered. For carbon steel the maximum operating temperature in the reactor is 538°C and for 304 SS, 310 SS or 316 SS the maximum operating temperature is 816°C.

**For your memo please provide the following information:**

- Description of the reactor system you think is best for this application.
- Material of Construction for any or all Reactors, heat exchangers and Fired Heaters
- Reactor Feed Temperatures and Reactor Exit Temperatures
- Ammonia Flow in kmol/hr leaving your reactor system. This is related to the single pass conversion, more ammonia flow = higher conversion.
- Total Bare Module Cost (CBM) for your reactor system including fired heater(s), S&T heat exchangers (if any), reactors and catalyst.

Please submit your Excel files and your Aspen Files into Canvas.

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Hints for Aspen Plus Simulation

Noting that the Ammonia molecule is polar. N₂ and H₂ are non-polar and the process is a high pressure process please use Exercise-02 PowerPoint to identify the thermo-package needed for this process simulation.

To make things simple for you please use zero pressure drop for all Aspen units.

To heat the process stream to the desired inlet temperature for reaction you can use Exchangers/Heater to determine the heat duty and then for costing purposes use a Fired Heater with the heat duty as the heater sizing factor.

For your reactor(s) please use Reactors/RPLUG. This reactor requires reaction stoichiometry and kinetics to be entered in a separate Reactions file block that is found near the bottom of the left-side Aspen Plus Simulation Panel just below the Utilities file block.

If you choose to use interstage coolers, they should be modeled and cost as shell and tube heat exchangers with an overall heat transfer coefficient of 250 BTU/hr/°F/ft² which will allow you to determine the heat exchanger area – the sizing factor. Make sure that the reactor outlet temperatures do not exceed the maximum temperature for your material of construction.

If you choose to use cold shots of feed between reactors, be careful to optimize the cold feed flows and watch for reactors with outlet temperatures that exceed the T_max for the material of construction.

If you choose a diluent, be careful to choose one that can be easily separated in the separation train and one that does not poison the iron catalyst. Any impurity with sulfur or phosphorus in it can poison the catalyst.