AMMONIA SYNTHESIS PLANT

Chemical Process Simulation Laboratory

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NOVEMBER 7, 2023

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1. Introduction

Ammonia, a remarkably versatile compound, holds a prominent role across diverse industries. In agriculture, it is a linchpin in the production of nitrogen-based fertilizers, fostering robust crop growth and enhancing agricultural yields. The refrigeration sector widely adopts ammonia as a refrigerant due to its efficiency and minimal environmental impact, aligning with a growing emphasis on eco-friendly practices.

Beyond agriculture and refrigeration, ammonia plays a pivotal role in various manufacturing processes. It is a key ingredient in the production of pharmaceuticals, plastics, and explosives, showcasing its adaptability across different sectors. The cleaning industry harnesses the power of ammonia for its effective degreasing and disinfecting properties, making it a stalwart in household cleaners.

In water treatment, ammonia contributes to maintaining optimal pH levels and aids in the removal of impurities, further expanding its utility. The widespread and diverse applications of ammonia underscore its significance, not just in industrial processes but also in meeting everyday needs across the spectrum of human activities.

2. Production of Ammonia

The Haber-Bosch process, a cornerstone of industrial chemistry, is the method by which ammonia, a crucial component in fertilizers, is synthesized from nitrogen and hydrogen. This groundbreaking process was developed by German chemists Fritz Haber and Carl Bosch in the early 20th century.

Ammonia (NH_3) is a vital compound in various industrial applications, but its primary demand arises in agriculture. It serves as a key component in the production of nitrogen-based fertilizers, playing a pivotal role in enhancing crop yields. Before the development of the Haber-Bosch process, ammonia was primarily obtained from natural sources or through less efficient chemical methods.

2.1 Basic Process

The heart of the Haber-Bosch process lies in the reaction between nitrogen (N_2) and hydrogen (H_2) to form ammonia (NH_3).

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

2.1.1 Nitrogen Extraction: The primary source of nitrogen for the process is the air we breathe, which is approximately 78% nitrogen. Extracting nitrogen from the air involves a series of steps. Air is first compressed to increase the concentration of nitrogen, and then cooled to liquefy it. The resulting liquid air is subjected to fractional distillation, a process that separates its components based on their different boiling points. Nitrogen, with a boiling point of -196℃ (-321 °F), is collected as a liquid.

2.1.2 Hydrogen Production: Hydrogen, on the other hand, is often derived from natural gas (methane) through a process called steam methane reforming. This method involves reacting methane with steam to produce hydrogen and carbon monoxide. The carbon monoxide is then further reacted with steam in a water-gas shift reaction to produce more hydrogen and carbon dioxide. The resulting hydrogen is purified to remove impurities before being used in the synthesis process.

2.1.3 Role of Catalysts: The Haber-Bosch process relies on catalysts to facilitate the reaction between nitrogen and hydrogen. Iron was chosen as the catalyst for its effectiveness and affordability. The process operates at elevated temperatures (around 450 degrees Celsius or 842 degrees Fahrenheit) and pressures (around 200 atmospheres), conditions necessary for the synthesis to proceed efficiently.

2.1.4 Reaction Mechanism: The Haber-Bosch process involves a dynamic equilibrium, meaning the reaction can proceed in both directions. The forward reaction forms ammonia, while the reverse reaction decomposes it back into nitrogen and hydrogen. Achieving a satisfactory yield of ammonia requires carefully balancing the reaction conditions.

2.2 Challenges and Optimization

2.2.1 Conversion: One of the challenges in the Haber-Bosch process is the slow rate of ammonia formation. The reaction is kinetically hindered, meaning it doesn't occur as rapidly as one might desire. To overcome this, high temperatures and pressures are employed. However, these conditions also pose challenges, as they require robust and expensive equipment to handle.

2.2.2 Energy Consumption: The process is known for its significant energy consumption. The compression of air, the synthesis of hydrogen, and the high-pressure conditions all contribute to the energy-intensive nature of the Haber-Bosch process. The need for efficient energy utilization and the exploration of alternative energy sources are ongoing areas of research to make the process more sustainable.

2.2.3 Impact on Agriculture: The development of the Haber-Bosch process had a profound impact on agriculture, leading to the mass production of synthetic fertilizers. This, in turn, revolutionized food production by providing a steady and abundant supply of nitrogen-based fertilizers. The increased availability of fertilizers contributed to the Green Revolution, a period of rapid agricultural development in the mid-20th century.

2.2.4 Environmental Considerations: While the process has played a crucial role in food production, it is not without environmental concerns. The production of ammonia results in the release of carbon dioxide and contributes to greenhouse gas emissions. Efforts are underway to develop more sustainable methods for ammonia synthesis, including research into alternative catalysts and the use of renewable energy sources.

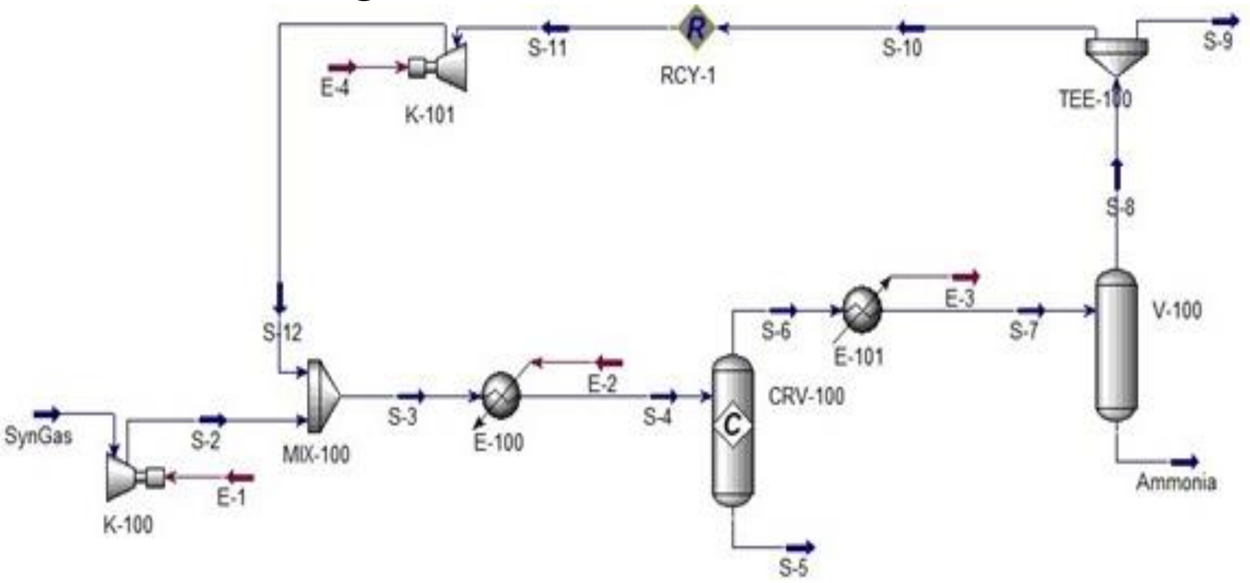
2.2.5 Ongoing Research and Future Prospects: Researchers continue to explore ways to improve the efficiency and sustainability of the Haber-Bosch process. This includes investigating novel catalysts, optimizing reaction conditions, and exploring alternative sources of nitrogen and hydrogen. Additionally, there is a growing interest in developing greener and more environmentally friendly methods for ammonia synthesis.

The Haber-Bosch process stands as a testament to human ingenuity in overcoming challenges to meet the needs of a growing population. Its impact on agriculture and food production cannot be overstated. However, as we move forward, the focus is not only on optimizing the existing process but also on developing new, sustainable approaches to ammonia synthesis. The story of the Haber-Bosch process is one of innovation, challenges, and the ongoing quest for solutions to feed a hungry world.

3. Process Condition and Specification

Syn-Gas Conditions		Temperature	280 °C
		Pressure	25.5 bar
		Molar Flowrate	7000 kg mole/hr
		Molar Compositions	
		N_2	0.2474
		H_2	0.7372
		CO	0.0024
		Ar	0.0027
		CH_4	0.0103
Equipment Specification			
Compressor 1	K-100	ΔP	249.5 bar
		Adiabatic Efficiency	75 %
Heater	E-100	Temperature	500 °C
		ΔP	0.1 bar
Conversion Reactor	CRV-100	Conversion	40 %
		Base Component	N_2
Cooler	E-101	Temperature	10 °C
		ΔP	100 bars
Purge Rate	TEE-100	1% of S-8 stream	
Compressor 2	K-101	ΔP	100.1 bar
		Adiabatic Efficiency	75 %

4. Process Flow Diagram



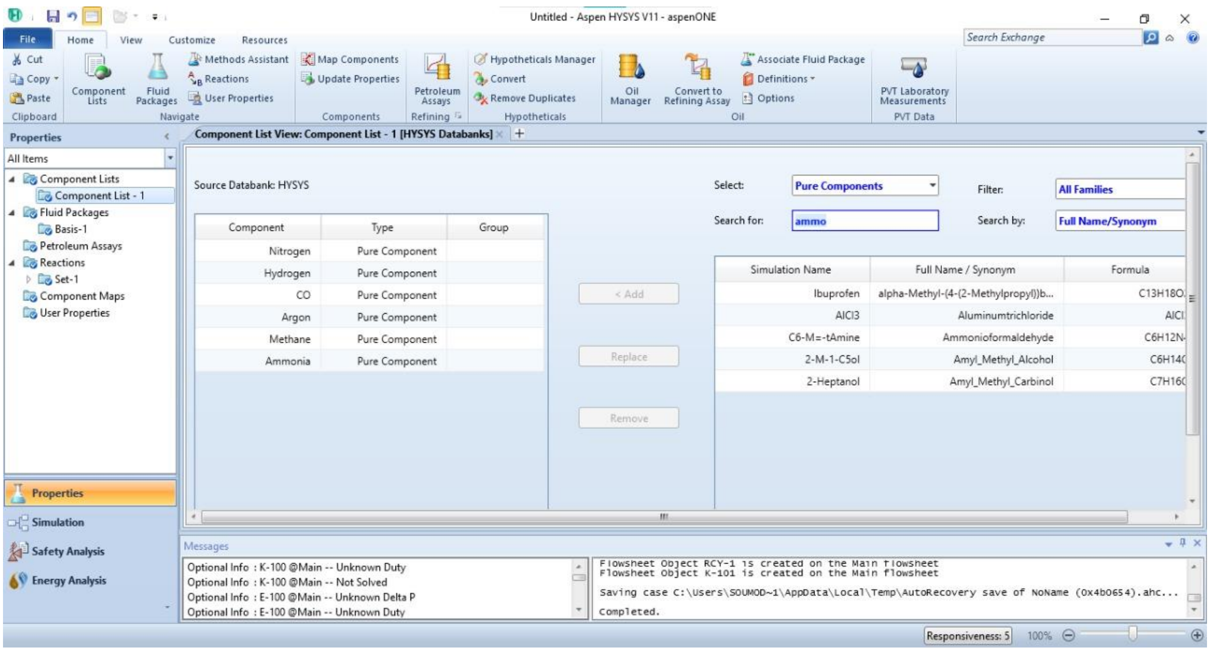
5. Process Simulation

The simulation of Ammonia Synthesis Plants in ASPEN HYSYS involves various steps. They are explained below.

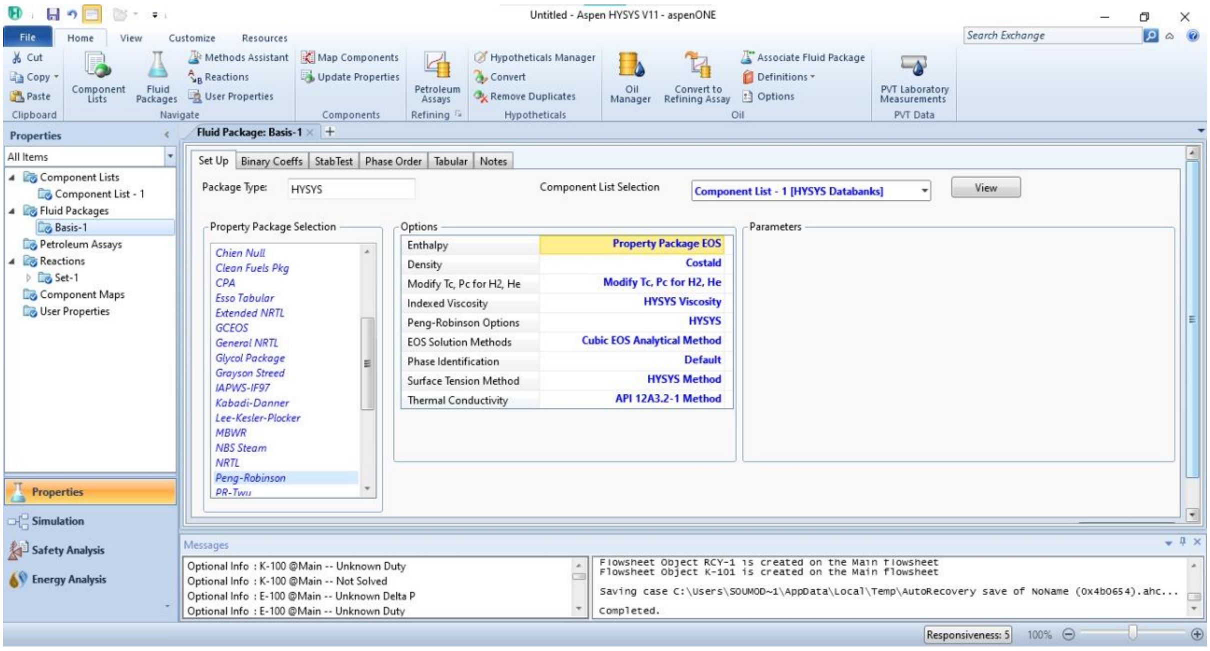
5.1 Defining Property Packages

First, we need to select all the components required for the plant simulation and required fluid packages. Also, we need to define the reactions taken place during the process.

5.1.1 Component Selection: We will select N_2, H_2, NH_3, CO, Ar & CH_4 as they all are involved in this process.



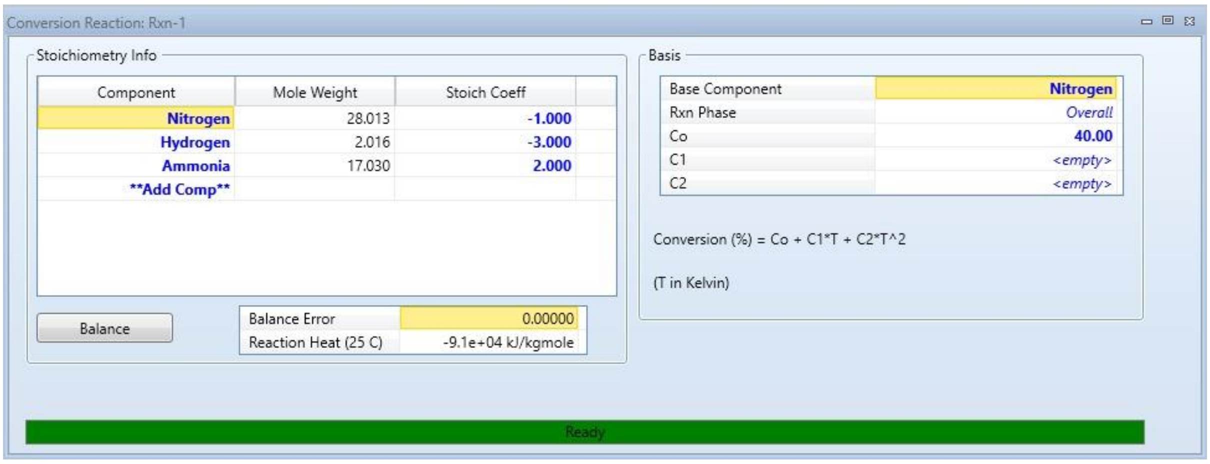
5.1.2 Fluid Package Selection: We will select the Peng-Robinson Fluid Package for this process.



5.1.3 Reaction Set Definition: Now we need to define the reaction involved in this process. Nitrogen and Hydrogen reacts to form Ammonia in this process.

$$N_2 + 3H_2 \leftrightharpoons 3NH_3$$

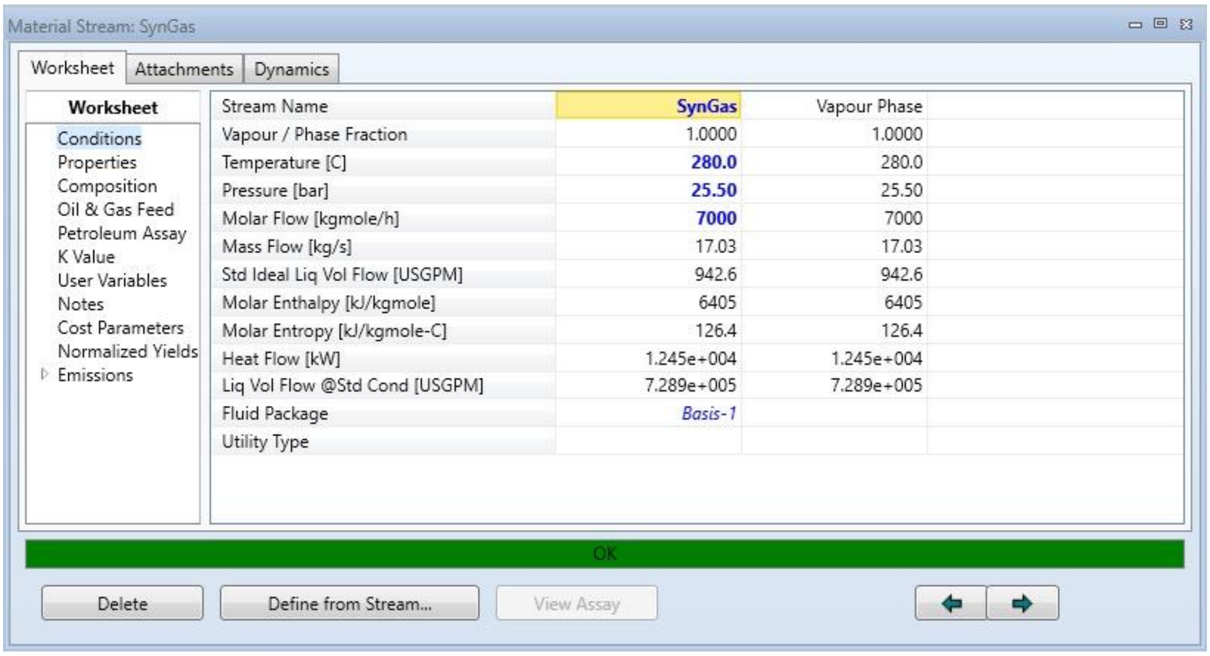
The Overall reaction results 40 % conversion based on Nitrogen. After defining the stoichiometric coefficients of all the components and the desired conversion, we will add the reaction to the Fluid Package.



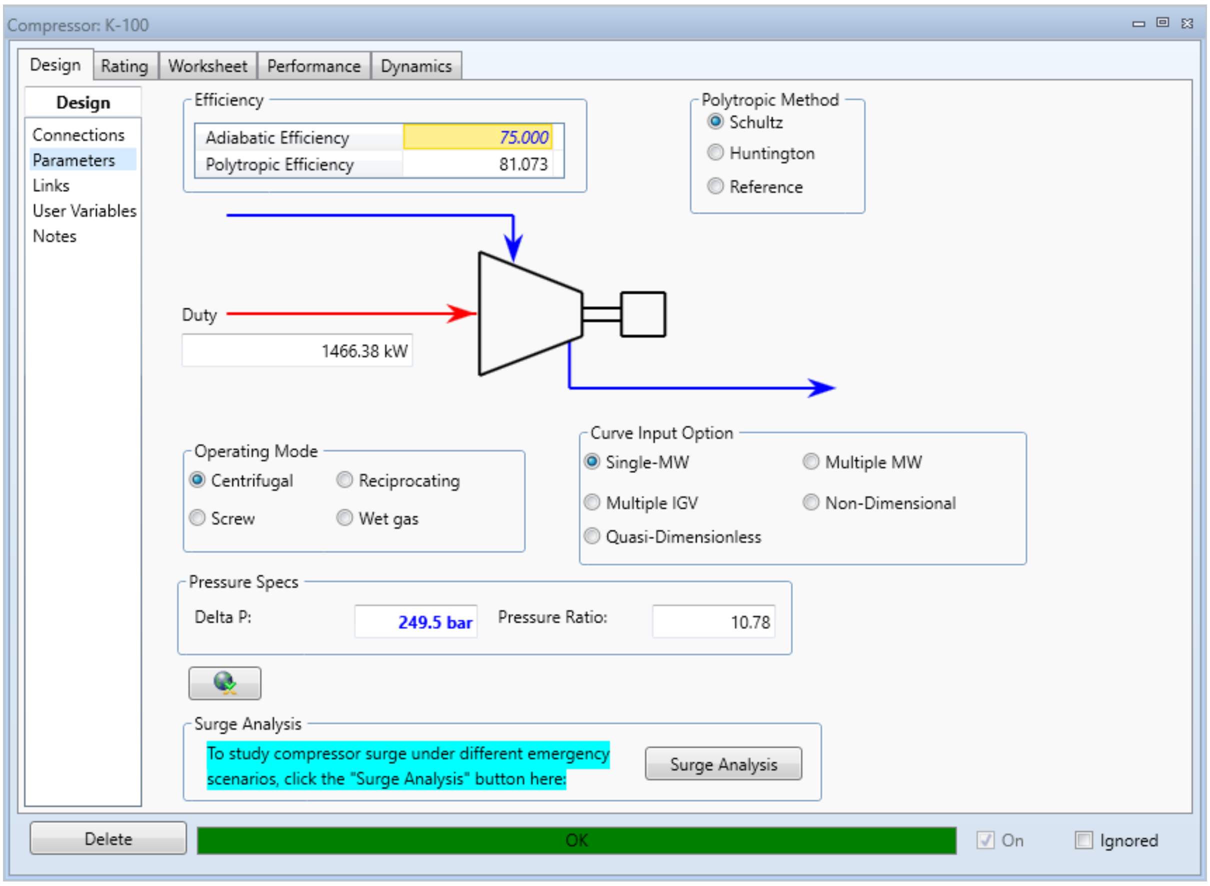
5.2 Simulating the Process

After Selecting all the Components, Fluid Packages and Reaction Set, now we start to simulate the process. Now, we will add all the equipment at specified condition to complete the whole simulation.

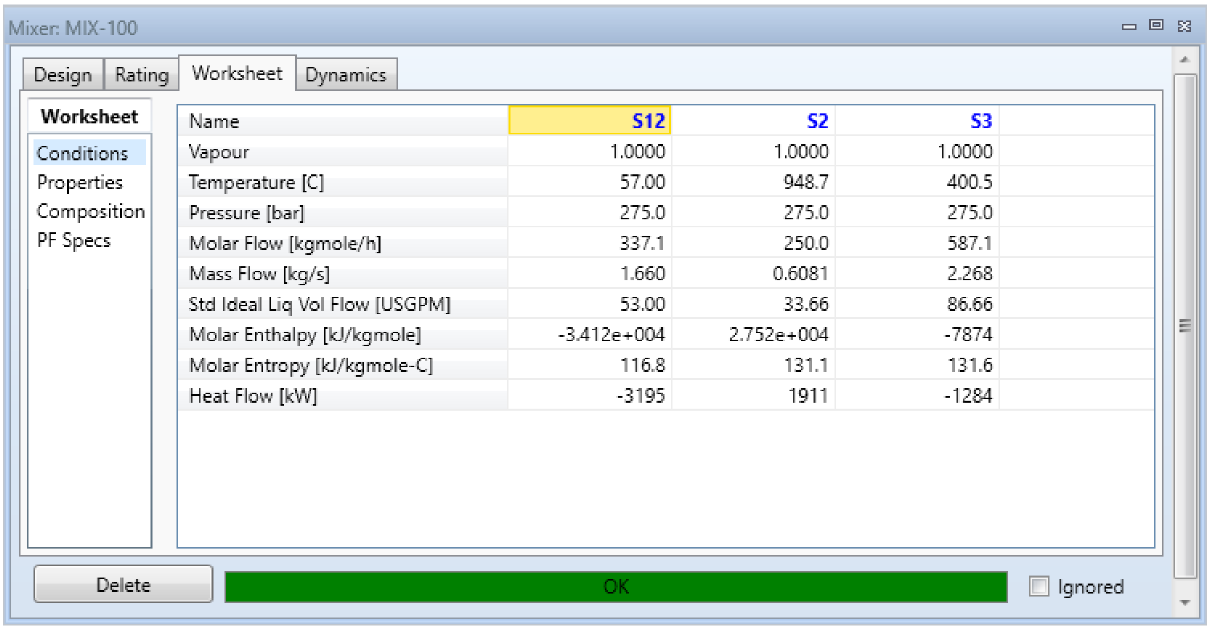
5.2.1 Defining Material Stream: First we will add the material stream named Syngas, and set the Temperature, Pressure and Molar Flowrate. After that, we will define the composition of the all component in the stream.



5.2.2 Compressor Specification: Now we will specify the Efficiency and the Pressure Difference of the compressor in the system.

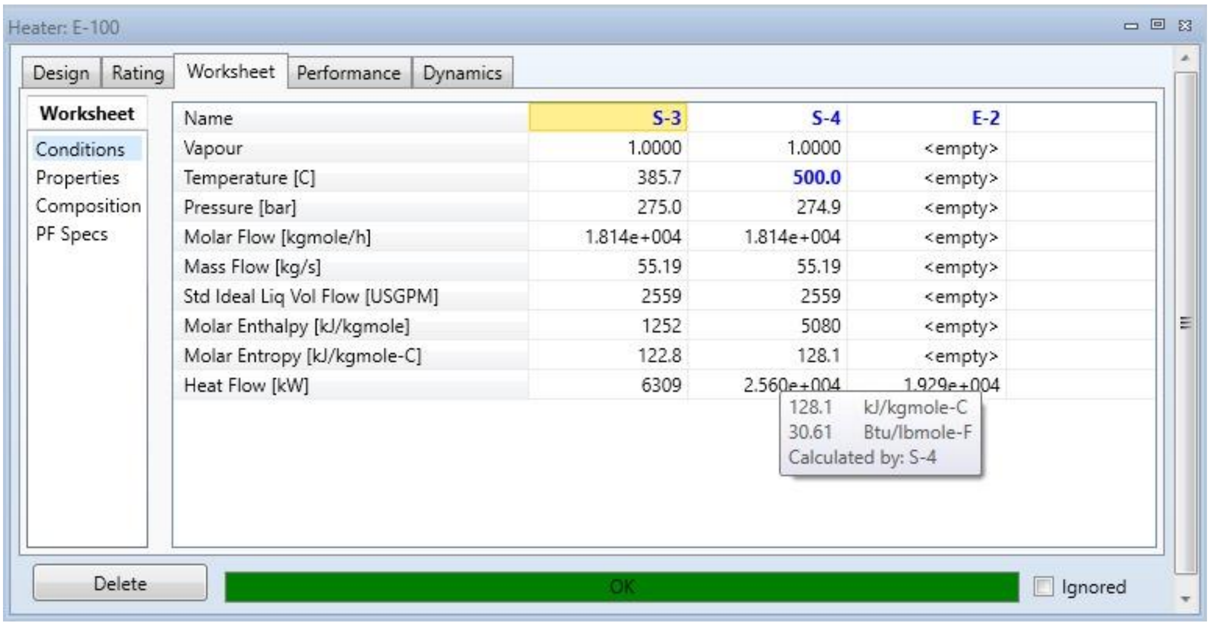


5.3.3 Mixer Specification: The compressed feed stream and the compressed recycle stream are mixed and sent to the heater for heating.



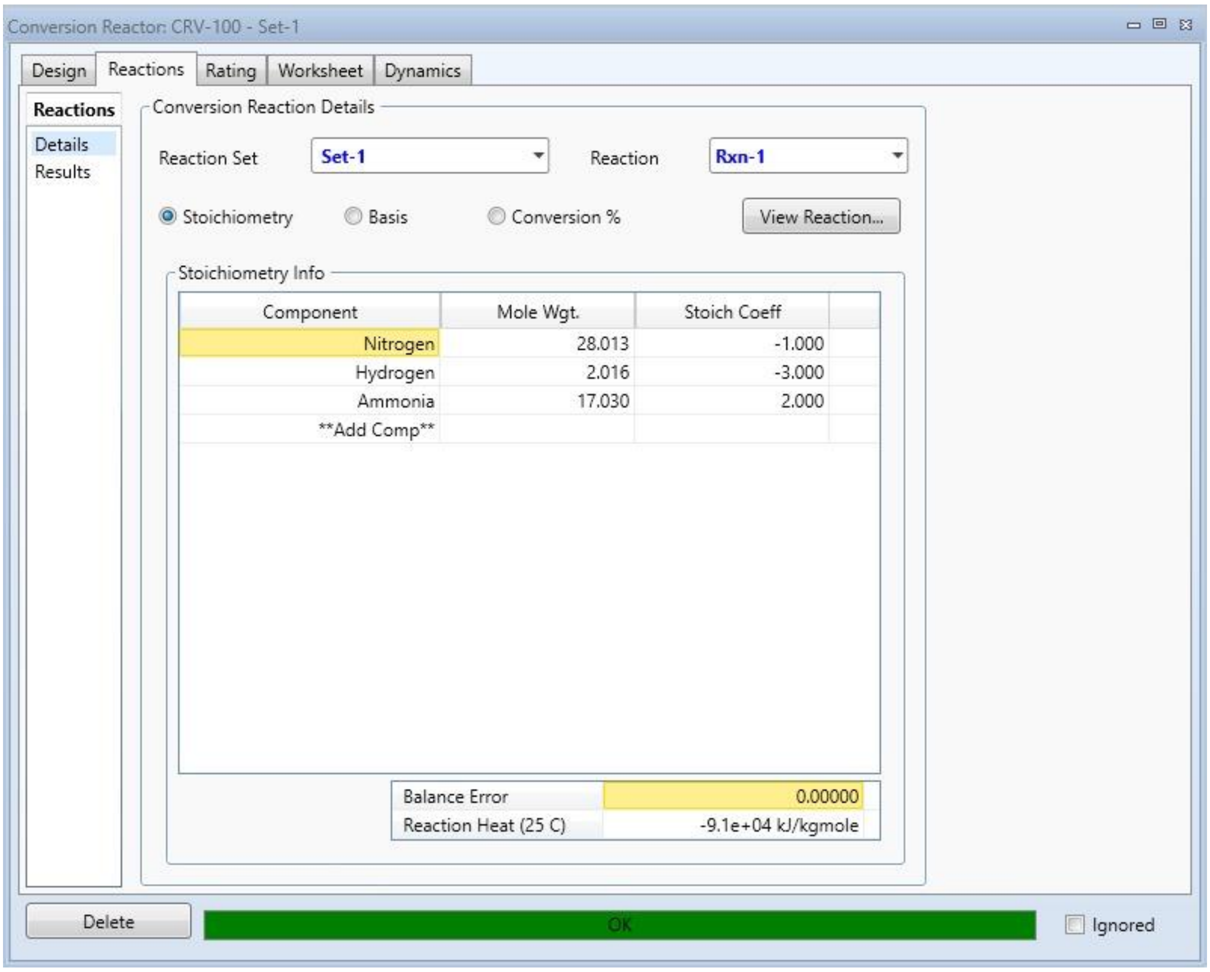
Name	S12	S2	S3
Vapour	1.0000	1.0000	1.0000
Temperature [C]	57.00	948.7	400.5
Pressure [bar]	275.0	275.0	275.0
Molar Flow [kgmole/h]	337.1	250.0	587.1
Mass Flow [kg/s]	1.660	0.6081	2.268
Std Ideal Liq Vol Flow [USGPM]	53.00	33.66	86.66
Molar Enthalpy [kJ/kgmole]	-3.412e+004	2.752e+004	-7874
Molar Entropy [kJ/kgmole-C]	116.8	131.1	131.6
Heat Flow [kW]	-3195	1911	-1284

5.3.4 Heater Specification: The mixture of fresh feed and recycle stream is heated up to 500℃ and a pressure drop of 0.1 *bar* is specified and the heated mixer is sent to the reactor.

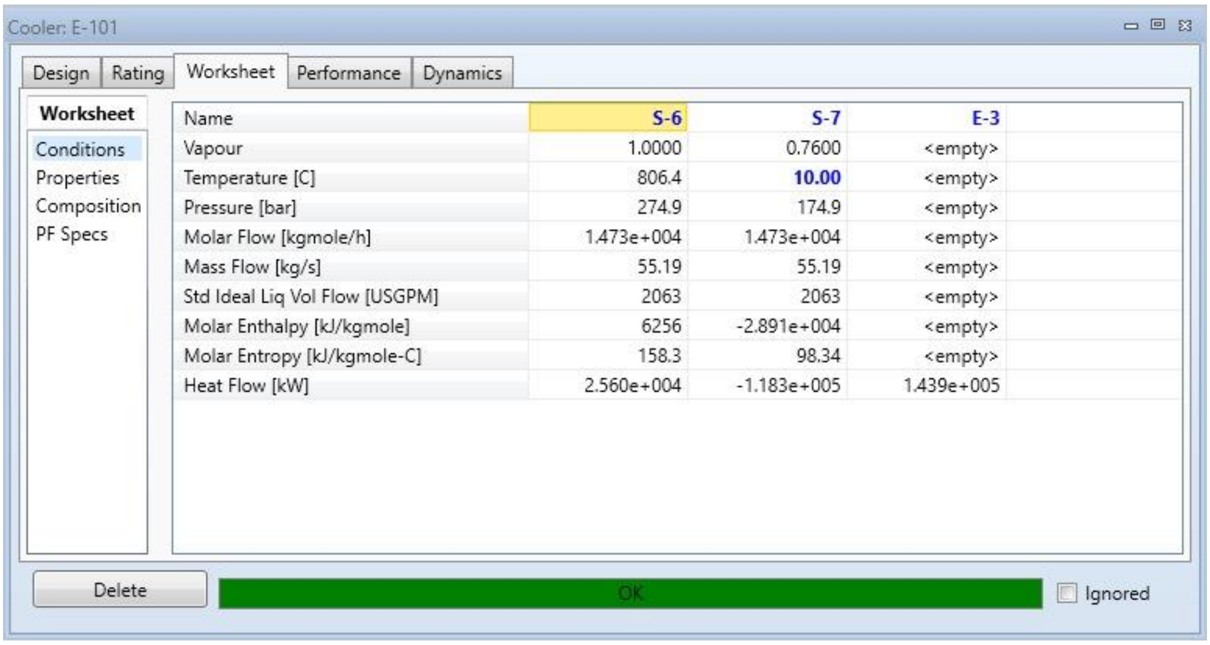


Name	S-3	S-4	E-2
Vapour	1.0000	1.0000	<empty>
Temperature [C]	385.7	500.0	<empty>
Pressure [bar]	275.0	274.9	<empty>
Molar Flow [kgmole/h]	1.814e+004	1.814e+004	<empty>
Mass Flow [kg/s]	55.19	55.19	<empty>
Std Ideal Liq Vol Flow [USGPM]	2559	2559	<empty>
Molar Enthalpy [kJ/kgmole]	1252	5080	<empty>
Molar Entropy [kJ/kgmole-C]	122.8	128.1	<empty>
Heat Flow [kW]	6309	2.560e+004	1.929e+004

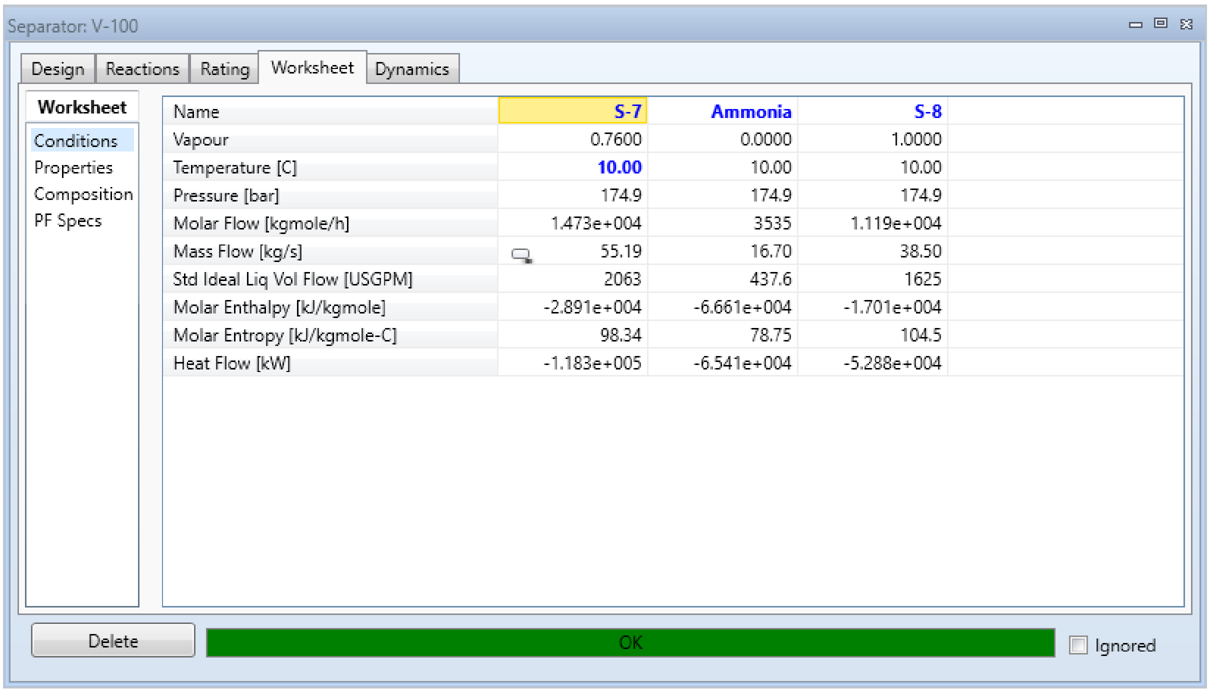
5.3.5 Reactor Specification: The feed mixture is sent to the reactor where the Ammonia is formed, and the conversion is 40% based on the Nitrogen.



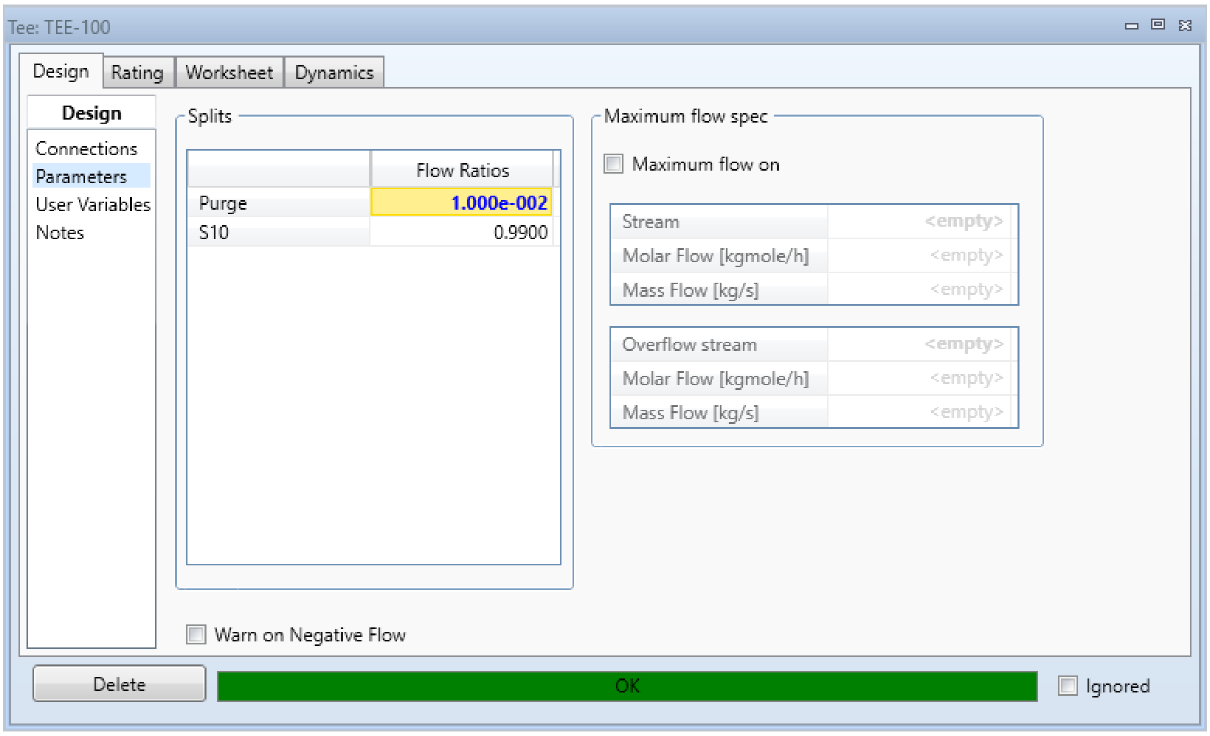
5.3.6 Cooler Specification: The output of the reactor is sent to the cooler where the mixture is cooled down to 10 ℃ where all the ammonia gets condensed, and the pressure is drastically reduced ($\Delta P \approx 100\ bar$).



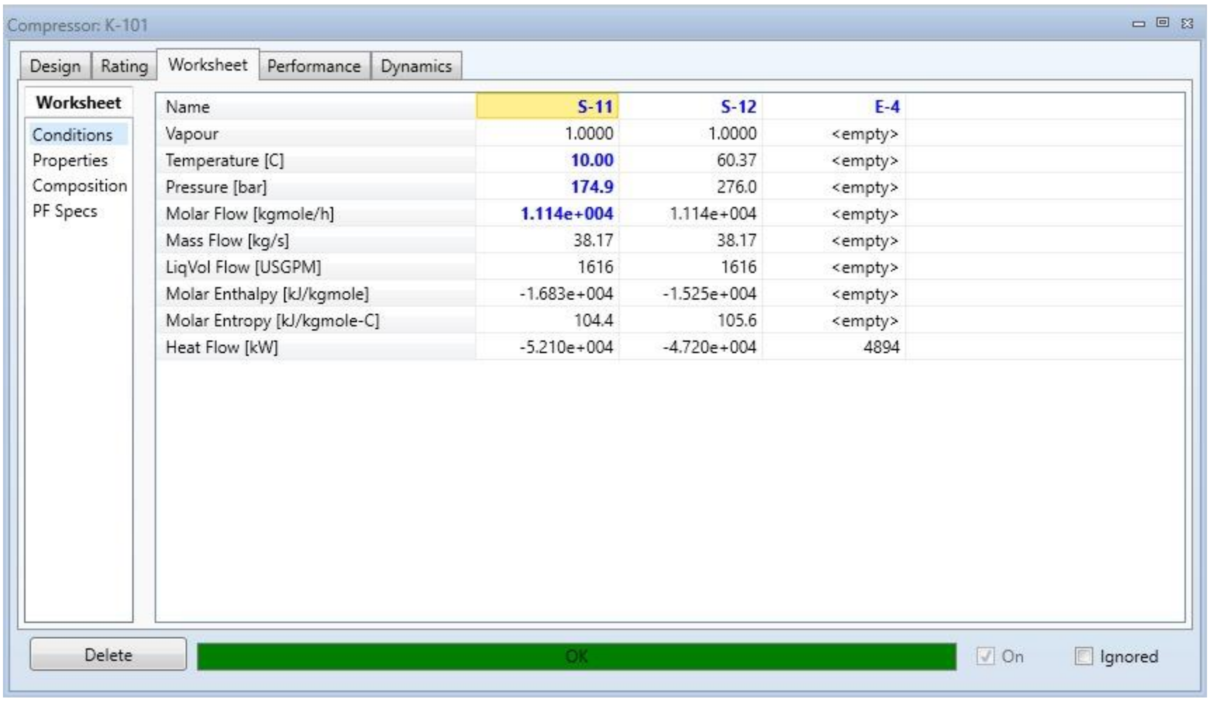
5.3.7 Separator: The cooled mixture is sent to the Separator where the liquified Ammonia is taken out and the gas mixture is sent to recycle back.



5.3.8 Splitter: 1% of the gas mixture is purged out and the rest is recycled and after compressing it is sent to the reactor again.



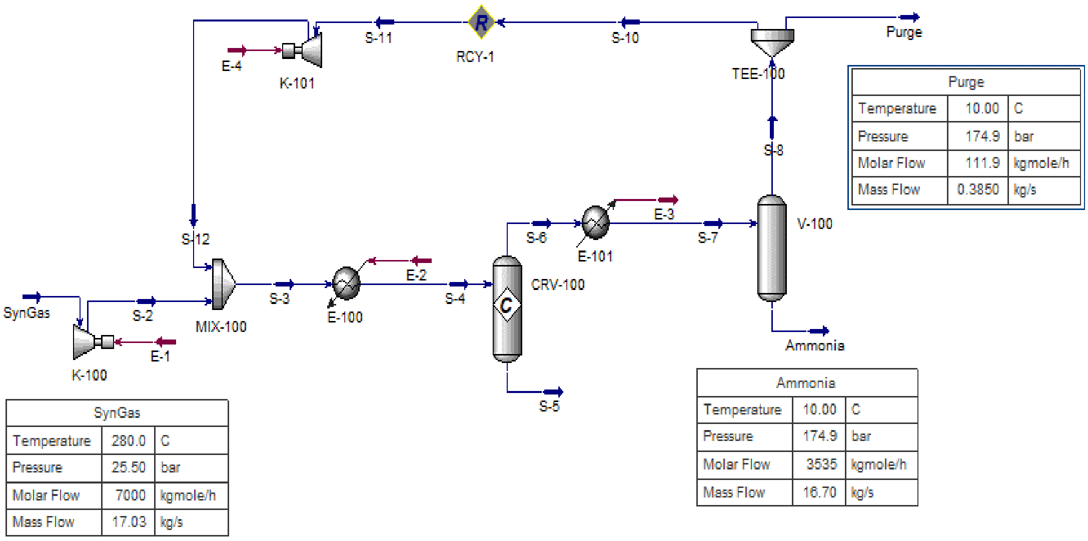
5.3.9 Recycle Compressor Specification: The recycled gas is sent to the compressor and is compressed up to 276 $bars$. This compressed gas stream is mixed with the feed and sent to the reactor.



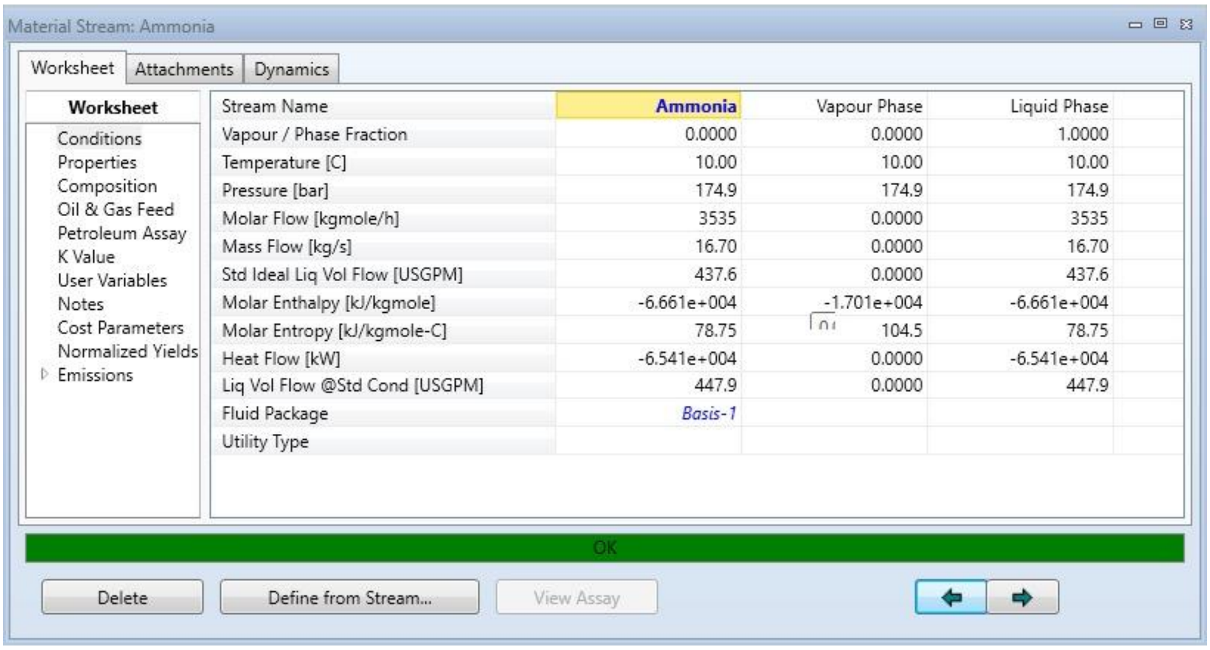
Name	S-11	S-12	E-4
Vapour	1.0000	1.0000	<empty>
Temperature [C]	10.00	60.37	<empty>
Pressure [bar]	174.9	276.0	<empty>
Molar Flow [kgmole/h]	1.114e+004	1.114e+004	<empty>
Mass Flow [kg/s]	38.17	38.17	<empty>
LiqVol Flow [USGPM]	1616	1616	<empty>
Molar Enthalpy [kJ/kgmole]	-1.683e+004	-1.525e+004	<empty>
Molar Entropy [kJ/kgmole-C]	104.4	105.6	<empty>
Heat Flow [kW]	-5.210e+004	-4.720e+004	4894

6. Result

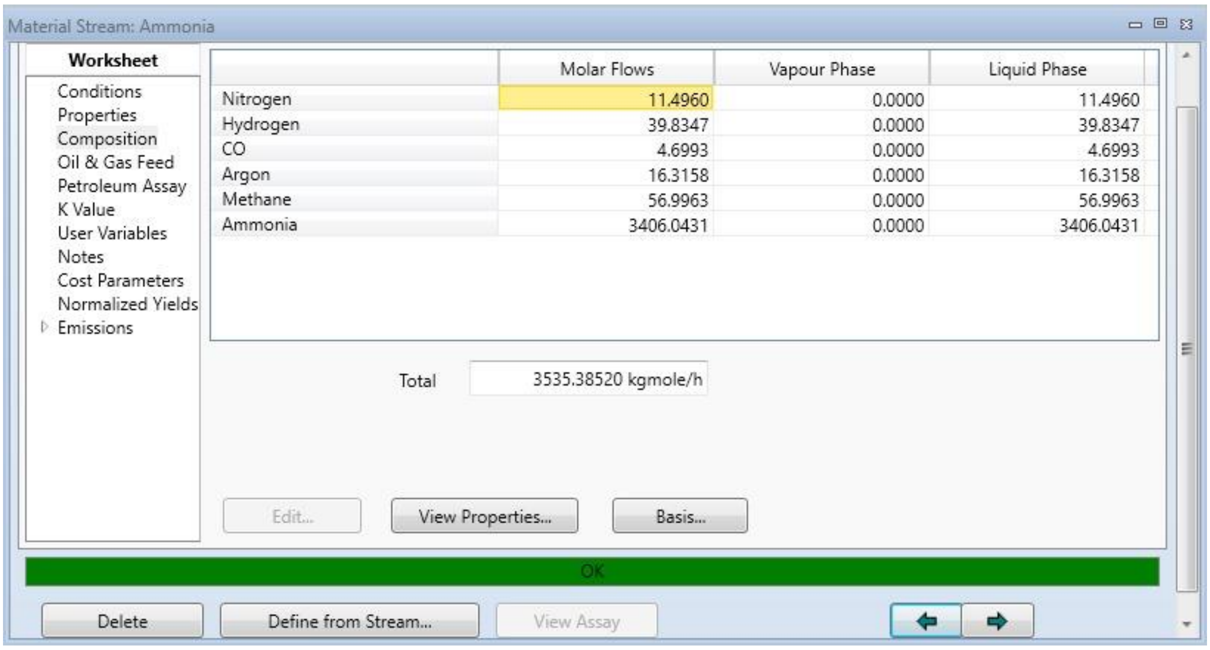
Now the final flowsheet is ready which is like the flowsheet given below.



For the given composition of the of the flowrate of 7000 $kgmole/hr$, The flowrate of the Ammonia stream will be 3535 $kgmol/hr$ (16.70 kg/s). The purity of the Ammonia stream is 96.34 %. The gas stream is split into 2 streams, 99 % is recycled back to the reactor and 1 % of the gas stream is purged out. The flowrate of the purge stream is 111.9 $kgmol/hr$ (0.385 kg/s). The purge gas contains 4.02% CO, 2.03% Ar & 10.58% CH_4. The Ammonia is taken out in liquid form.

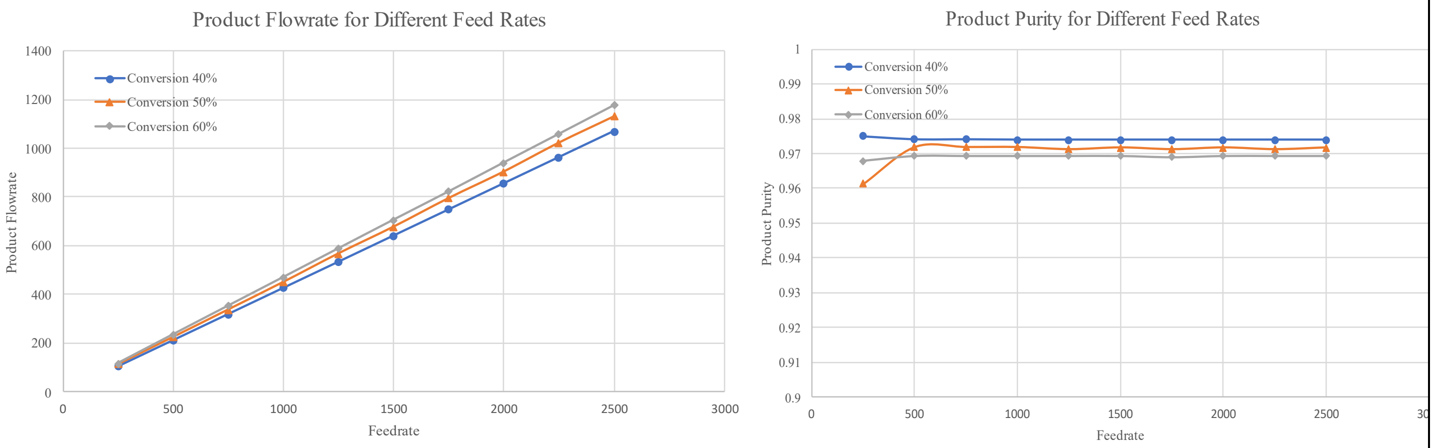


Stream Name	Ammonia	Vapour Phase	Liquid Phase
Vapour / Phase Fraction	0.0000	0.0000	1.0000
Temperature [C]	10.00	10.00	10.00
Pressure [bar]	174.9	174.9	174.9
Molar Flow [kgmole/h]	3535	0.0000	3535
Mass Flow [kg/s]	16.70	0.0000	16.70
Std Ideal Liq Vol Flow [USGPM]	437.6	0.0000	437.6
Molar Enthalpy [kJ/kgmole]	-6.661e+004	-1.701e+004	-6.661e+004
Molar Entropy [kJ/kgmole-C]	78.75	104.5	78.75
Heat Flow [kW]	-6.541e+004	0.0000	-6.541e+004
Liq Vol Flow @Std Cond [USGPM]	447.9	0.0000	447.9
Fluid Package	Basis-1		
Utility Type			

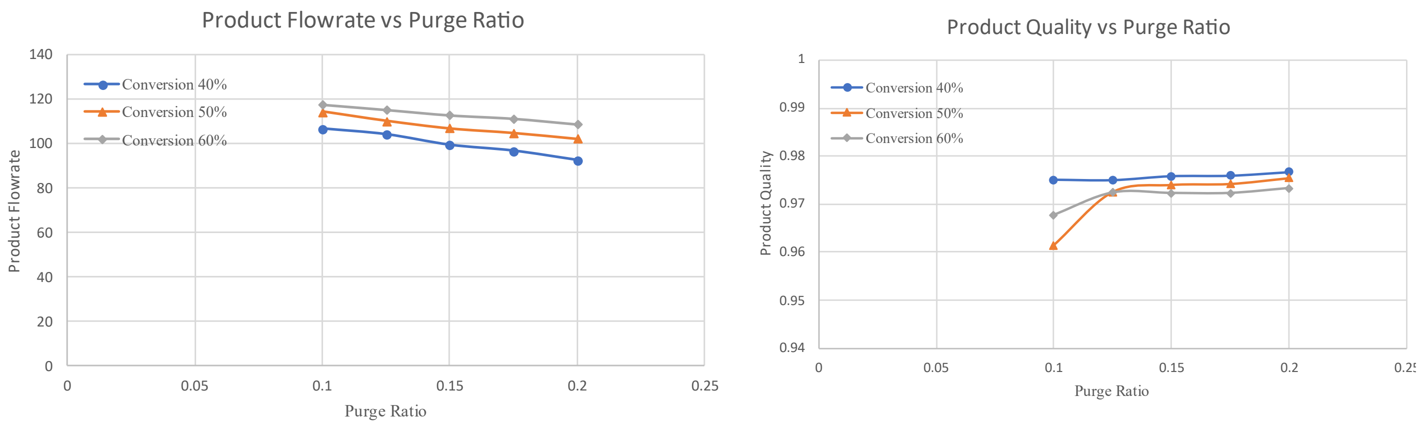


	Molar Flows	Vapour Phase	Liquid Phase
Nitrogen	11.4960	0.0000	11.4960
Hydrogen	39.8347	0.0000	39.8347
CO	4.6993	0.0000	4.6993
Argon	16.3158	0.0000	16.3158
Methane	56.9963	0.0000	56.9963
Ammonia	3406.0431	0.0000	3406.0431

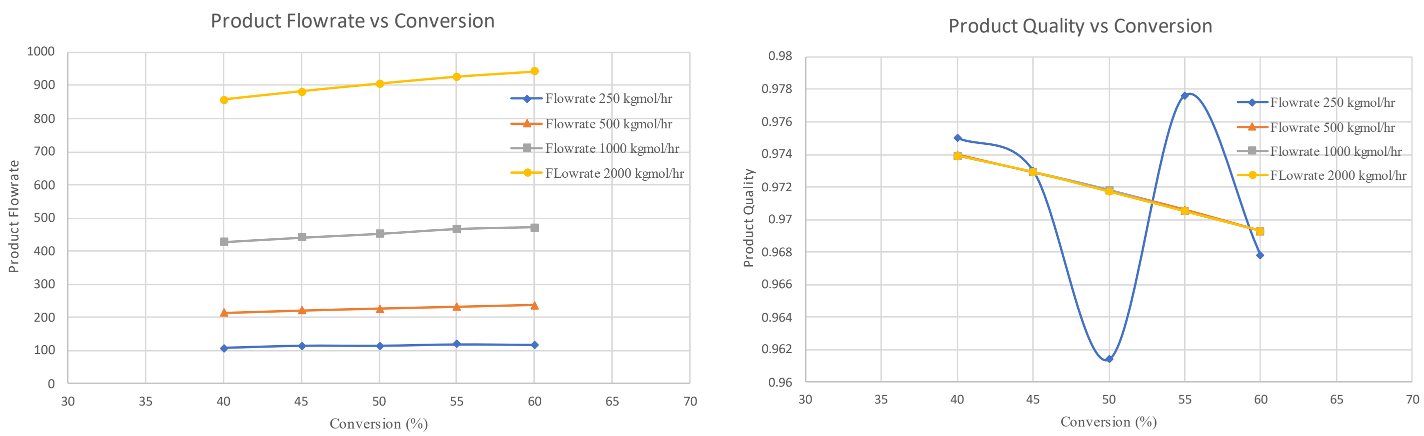
The quality and production of the Ammonia depends on the Purge Ratio, Feed Rate, and the Conversion of the reactions. The following graph shows the relationship between those quantities.



Variation of product flowrate and product purity at different flowrate and purge ratio of 1 %



Variation of product flowrate and product purity at different purge ratio and Flow rate of 250 kg mole/hr



Variation of product flowrate and product purity at different Conversion Rate and Purge ratio of 1 %

7. Discussion

From the graph we can easily observe that if we increase the Feed flowrate the product flowrate will increase whereas the product quality dose not affected, almost remains constant. Also, if we increase the purge the ratio, the product flowrate decreases but it has no significant impact on the product quality. Whereas, if we increase the conversion in the reactor, The product flowrate increases but the quality of the product decreases. So, need a trade-off between them.