

Simulation of Ammonia Production using HYSYS Software

Prof. /Nabil Abdel El Moneim
Cairo University, Faculty of Engineering

Prof. / Ibrahim Ismail
Cairo University, Faculty of Engineering

Nasser. M.M
Egyptian Armed Force.

Abstract

Now-a-days, Because of cost and time consuming in the design of plants chemical engineer used simulators to simulate design and operation of chemical equipment and plant, which spares a great deal of time and cash. Today, there are many number of the simulators are refreshed and utilized in the simulation of chemical equipment and plant such as ChemCad, ProII, UniSim.....etc. Among of these simulators, Aspen Hysys is the most utilized programming in all ventures because of aiding in two noteworthy fields (design & operation). Simulation of ammonia synthesis process is done on Aspen Hysys V8.8 with steady state mode making some assumptions and using hypothetical reactors ammonia. By fluctuating the distinctive parameters in this simulation environment, the impact of these parameters in the generation rate of the procedure are watched.

Keywords: Ammonia, Simulation, Aspen Hysys

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1. Introduction

Ammonia is a compound of nitrogen and hydrogen with the recipe NH_3 . It is a drab gas with a trademark sharp smell. [1]

Ammonia is used in the Production of nitrogen fertilizers as the primary element. Ammonia is used in a plenty of application such as used as a fertilizer or used as a feedstock in synthesis of many compounds such as urea, or nitric acid, etc. [2] The demands for ammonia production are increased due to higher world's consumption of ammonia in synthetic fertilizers. [3]

Haber-Bosch process [4] is the main industrial method for ammonia production which created in 1905 by Fritz Haber and developed for industry in 1910 by Carl Bosch. In Haber-Bosch process, the reaction between nitrogen and hydrogen lead to produce ammonia in the presence of iron catalysts and at a high pressure and temperature.

In Haber-Bosch process, 150 million tons of ammonia is produced yearly which is approximately five times higher than produced before Haber-Bosch process. In ammonia synthesis, production of hydrogen is from natural gas and production of nitrogen is from atmospheric air. [2,5]

Simulation is used to simulate the operation of both state steady state (time is ignored) and dynamic state (time isn't ignored). Simulation is also used to display the courses of action and actually effects of other conditions.

Aspen Hysys [6] is generally used for process of oil and gas industry but it's expanded to simulation of various industries such as Oil refinery, Sweetening of Acid Gas with DEA, Industries of Heavy chemical, Industries of Petrochemical, Plant of Natural gas process, Industries of Petroleum,.....etc.

The property package in HYSYS can display exact thermodynamic and physical property forecasts for hydrocarbon, non-hydrocarbon, chemical fluids and petrochemical. The database of Hysys contains many components exactly more than 1500 components and over 16000 fitted binary coefficients and the creation of hypothetical components is performed when the database doesn't contain any components. [7]

Presently a-days, simulators are used for different chemical engineering purposes for example, outline new plants, diminish capital expenses for plant, huge monetary advantages for the procedure, and so on. Though our task was to represent production of ammonia in aspen HYSYS software v 8.8, making a few suppositions and utilizing theoretical reactors ammonia production simulation have been performed with the steady state behavior of the process.

2. Methodology:

In this paper, ammonia production plant was simulated by using one of the best chemical engineering simulators, called ASPEN HYSYS (V8.8) with steady state mode.

2.1 Process Description:

The process of ammonia production depended on two basic parts: Production of syngas and Production of ammonia. The production of syngas contains a lot of unit operations as the following: (1) steam reforming (primary reforming) which is responsible for producing hydrogen, (2) air reforming (secondary reforming) which is used to generate nitrogen, (3) High& Low shift conversion which is used to convert all carbon monoxide to carbon dioxide, (4) CO₂ removal and(5) methanation.

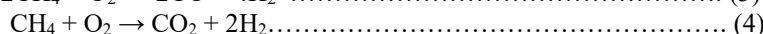
2.1.1 Hydrogen Production:

Hydrogen is predominantly generated from the reaction amongst methane and steam. Natural gas is sent to the primary reformer for steam reforming, where superheated steam is fed into the reformer with the methane at 639.7°C in the presence of a nickel catalyst where methane is changed over to hydrogen, carbon dioxide and little amounts of carbon monoxide.



2.1.2 Nitrogen addition:

The synthesis gas from primary reformer is sent to the secondary reformer where syngas blended with air within the sight of profoundly exothermic reaction amongst oxygen and methane produces more hydrogen. What's more, the important nitrogen is included in the secondary reformer



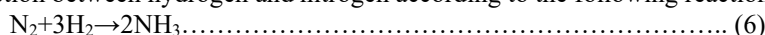
2.1.3 Removal of carbon monoxide & carbon dioxide:

It is essential advance to expel carbon dioxide and staying of carbon monoxide with a specific end goal to keep the toxin of ammonia synthesis reaction. At high temperature shift conversion, carbon monoxide is changed over to carbon dioxide at 583°C and likewise carbon monoxide is expelled and changed over to carbon dioxide at low temperature move change (325°C).



2.1.4 Ammonia Production:

Ammonia is produced due to reaction between hydrogen and nitrogen according to the following reaction:



2.2 Equipment & Software:

The software used in the simulation of ammonia plant design is Aspen Hysys (v.8.8) with steady state mode. The equipments used from aspen Hysys in the simulation of ammonia plant design are shown in Table (1).

Table (1) Equipment used in the simulation of ammonia plant design

Equipment used in the simulation	Coolers & Mixers	CO ₂ absorber	Compressors
	Low temperature shift conversion reactor (LTSC)	High temperature shift conversion reactor (HTSC)	Ammonia converter reactor
	Primary & Secondary reformer	Methanator reactor	separators

2.3 Simulation of the process:

The main steps for ammonia process simulation by using aspen hysys are the following:

- 1) Selection of component list.
- 2) Selection of fluid package.
- 3) Defining reactions and formation of reaction sets.
- 4) Installing the feed streams
- 5) drawing flow sheet.

Fig (15) shows the Process Flow Diagram (PFD) for the production of ammonia process, generated by Aspen HYSYS.

2.3.1 Selection of components list:

In this simulation, the reactant component list contain CH₄, H₂O, CO, CO₂, N₂, H₂, O₂ ignoring sulfur content as the components for the ammonia production. Figure (01) demonstrates the used component list in aspen hysys programming.

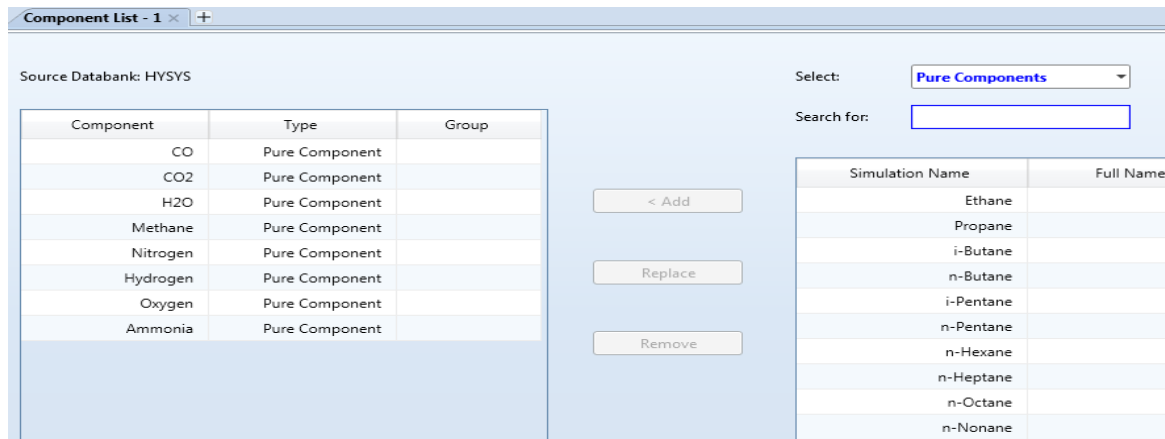


Figure (01) component list in aspen hysys software

2.3.2 Selection of fluid package:

In this simulation, the used fluid package is Peng- Robinson (PR), which is the most improved model in Aspen HYSYS.

2.3.3 Defining reactions and formation of reaction sets:

In this simulation, the procedure of ammonia production involves sets of reactions; primary reforming, secondary reforming, high and low shift conversion, methanation, ammonia converter. Figures from (02) to (07) give input information to the making of different reactions sets.

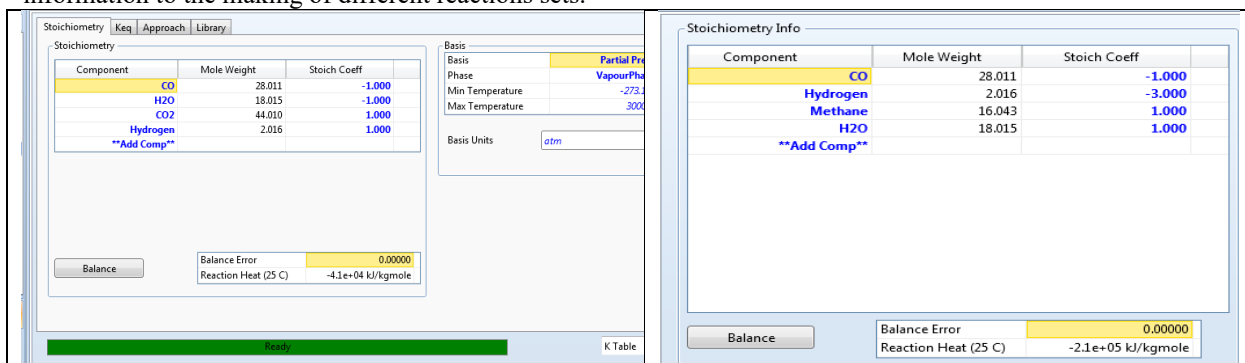


Figure (02) design the reaction (set-1) of HTSC & LTSC reactor.

Figure (03) design the reaction (set-2) of Methanator reactor.

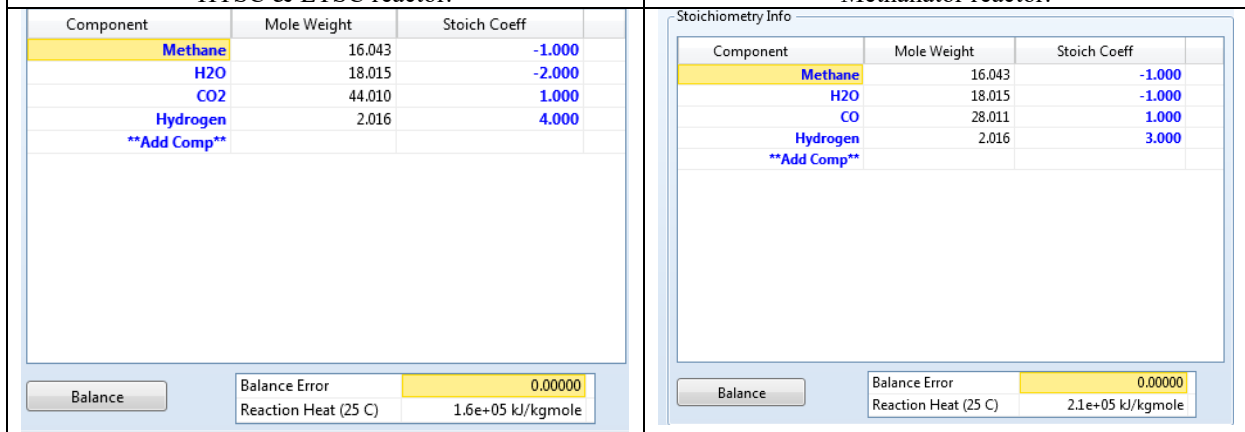


Figure (04) design the reaction (set-3) of first reformer.

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
CO2	44.010	1.000
H2O	18.015	2.000
Oxygen	32.000	-2.000
Add Comp		

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-2.000
CO2	44.010	1.000
Hydrogen	2.016	4.000
Add Comp		

Balance Error: 0.00000
 Reaction Heat (25 C): -8.0e+05 kJ/kgmole

Figure (05) design the reaction (set-4) of second reformer.

Component	Mole Weight	Stoich Coeff
CO2	44.010	-1.000
Hydrogen	2.016	-4.000
Methane	16.043	1.000
H2O	18.015	2.000
Add Comp		

Component	Mole Weight	Stoich Coeff
Hydrogen	2.016	-3.000
Nitrogen	28.013	-1.000
Ammonia	17.030	2.000
Add Comp		

Balance Error: 0.00000
 Reaction Heat (25 C): -1.6e+05 kJ/kgmole

Figure (06) design the reaction (set-5) of methanator (1) reactor

Figure (07) design the reaction (set-6) of ammonia converter reactor

2.3.4 Installing the feed streams:

Natural gas & steam are the feed streams for the primary reformer. A stream of air is associated with the secondary reformer. For these streams, it is vital to characterize this properties temperature, pressure, and component mole fraction as appeared in table (2).

Table (2) the basic streams conditions for the simulation

Stream	Temperature (°C)	Pressure (Kpa)	Component mole fraction						
			Ch4	H ₂ O	CO	CO ₂	H ₂	N ₂	O ₂
R-LNG	371	3346	0.985	0	0	0.0008	0	0.0142	0
Steam	246.1	3445	0	1	0	0	0	0	0
Air	30	3445	0	0	0	0	0	0.79	0.21

3. Result and Discussions:

After performing the simulation, the influence of different processing parameters such as (temperature and pressure of steam, temperature and pressure of natural gas ... etc) on the production rate of the process are observed & by controlling these parameters optimum ammonia production can be obtained. From the simulation result, those effects are described in below.

3.1 Temperature of natural gas:

From the figure (08), it is observed that the influence of temperature of natural gas on ammonia product rate as the increases of the temperature of natural gas cause decrease of ammonia production rate.

3.2 Pressure of natural gas:

From the figure (09), influence of the pressure of natural gas on ammonia production rate is observed where from interval 1000 kpa to 3000 kpa the increases of the pressure cause decrease of ammonia production rate & from higher than 3000 kpa the increase of the pressure cause slightly increase of ammonia production rate.

3.3 Temperature of steam:

From the the figure (10), the influence of temperature of steam on ammonia production rate is very clear in three intervals as from 200-250 °K the increase of the temperature cause increase of the ammonia production rate & from 250-300 °K the maximum ammonia production rate is obtained & from higher than 300 °K the increase of temperature cause decrease of ammonia production rate so the optimum operating temperature of steam is from 250-300 °K.

3.4 Pressure of steam:

From the figure (11), it is observed that the influence of Pressure of steam on ammonia product where the increase of pressure of steam cause increase of the ammonia production rate.

3.5 Temperature of air:

From the figure (12), the influence of the temperature of air is very clear where the increases of temperature of air cause decrease of the production rate.

3.6 Pressure of air:

From the figure (13), it is seen that the increase of the pressure of air cause increase on the production rate.

3.7 temperature of the feed (hydrogen & nitrogen)

From the figure (14), it is seen that the increase of the feed temperature cause decrease of the ammonia production rate.

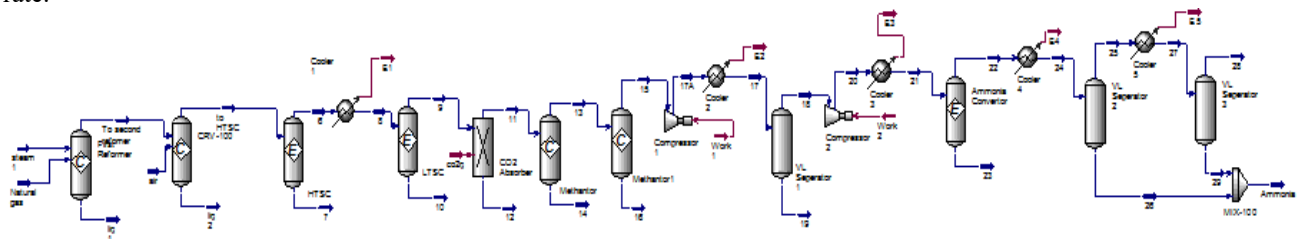


Figure (15) Hysys Process Flow diagram of ammonia synthesis

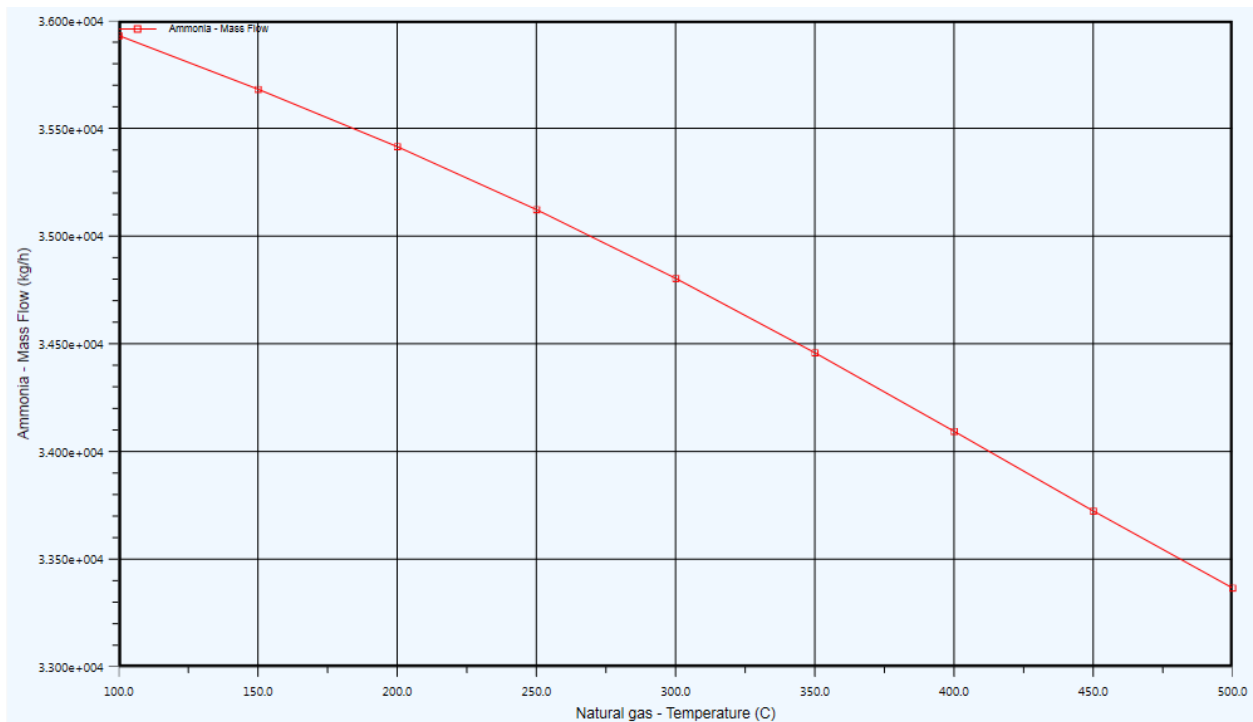


Figure 08: temperature of natural gas vs. Mass flow rate of ammonia

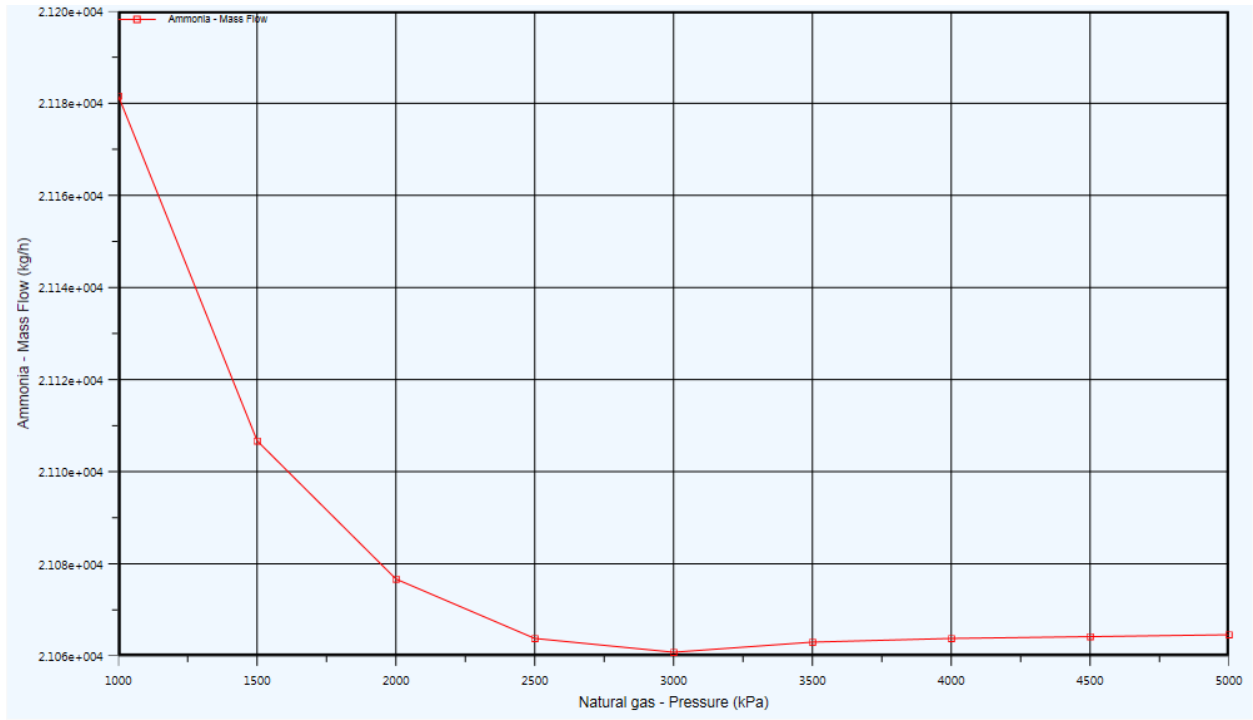


Figure 09: pressure of natural gas vs. Mass flow rate of ammonia

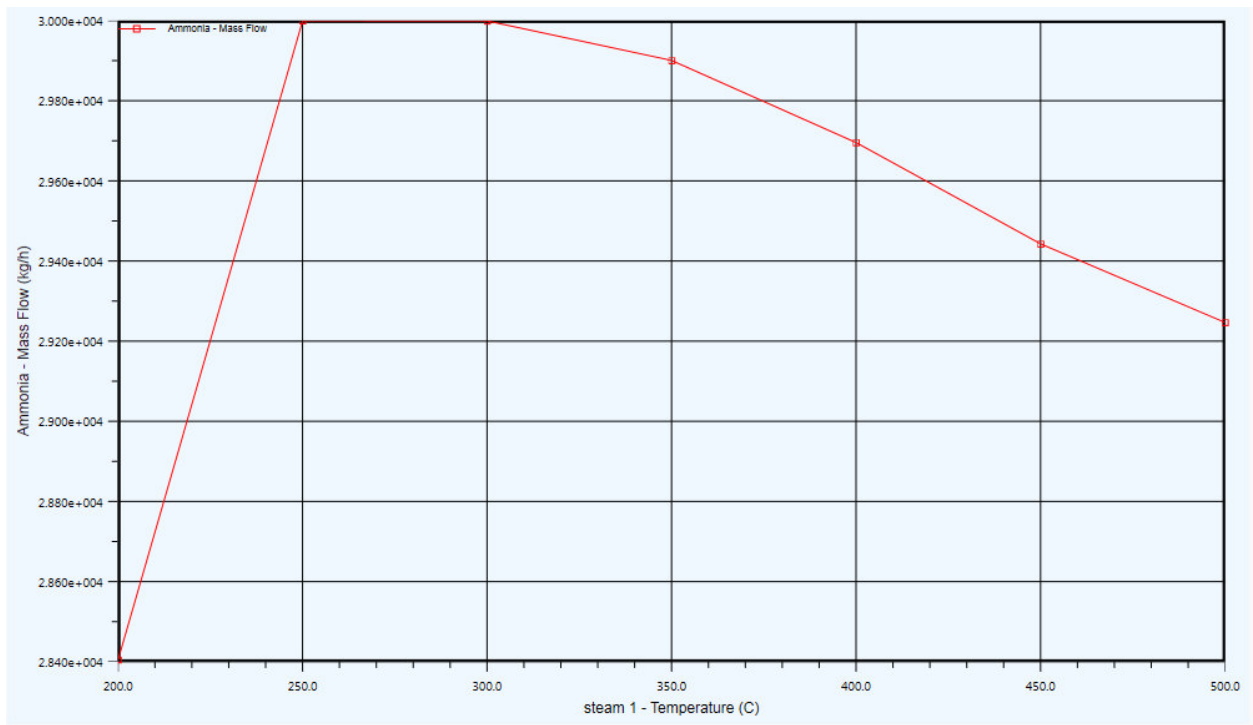


Figure 10: temperature of steam vs. Mass flow rate of produced ammonia.

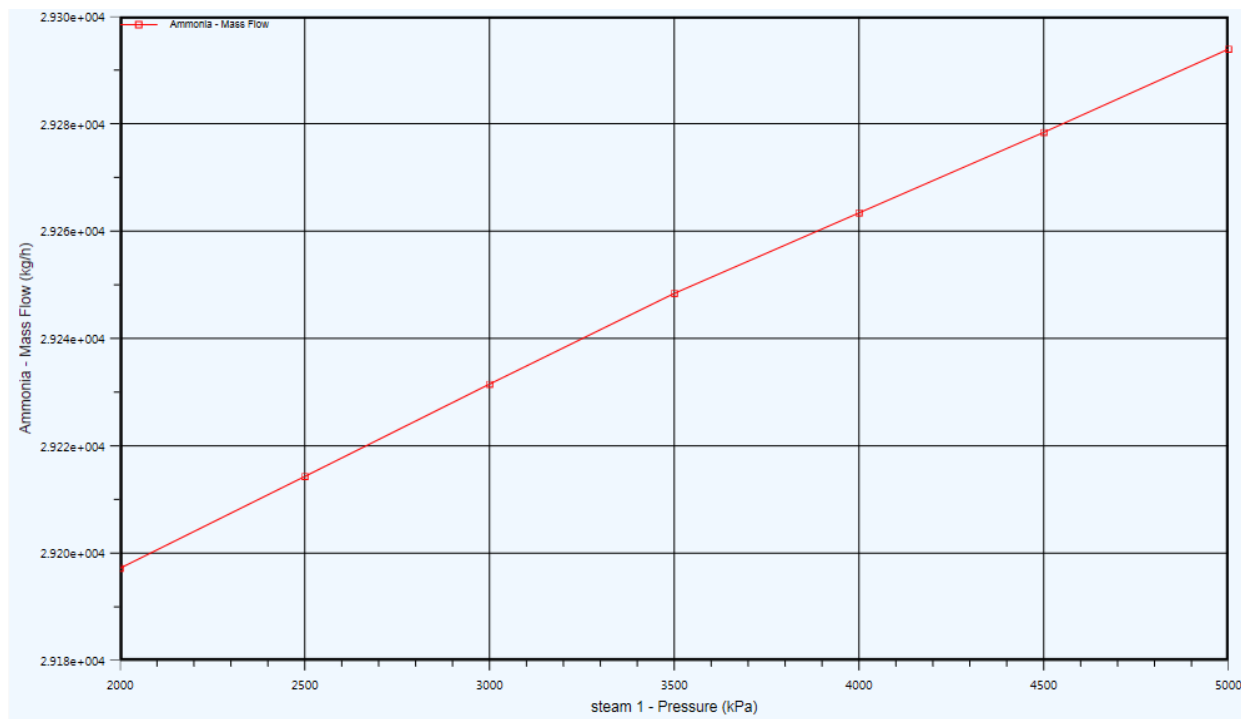


Figure 11: pressure of steam vs. Mass flow rate of produced ammonia.

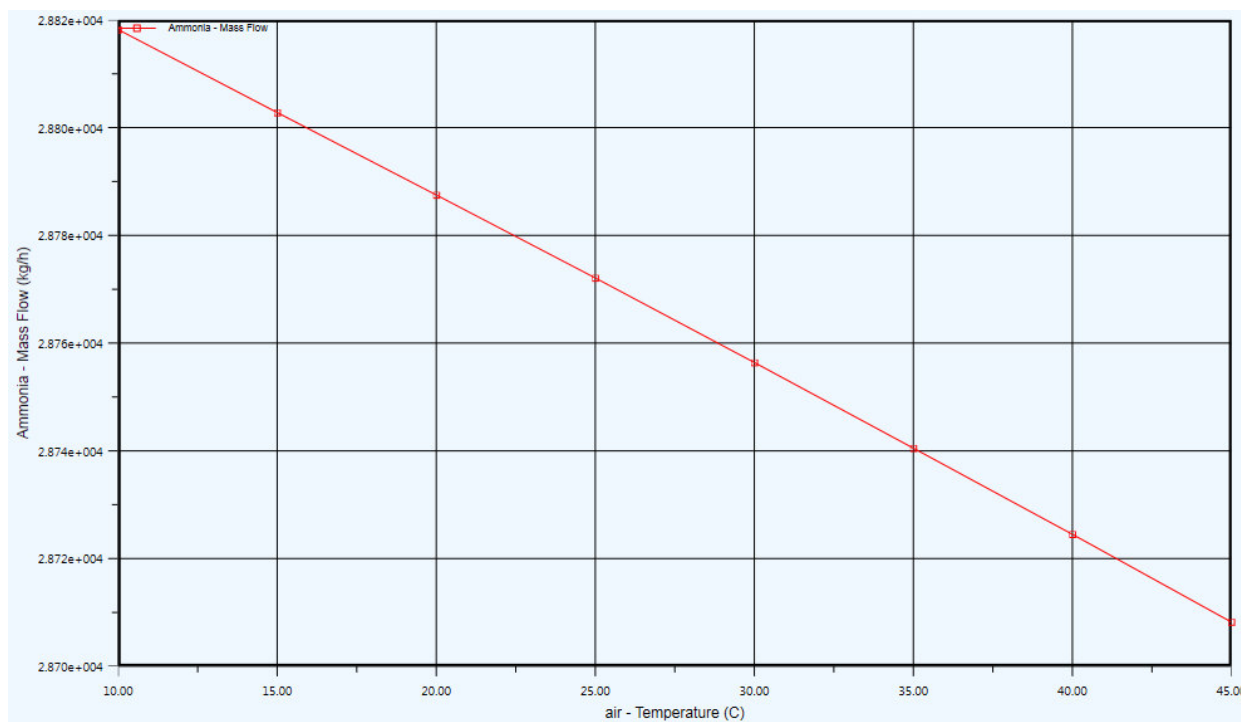


Figure 12: Temperature of feed of air vs. Mass flow rate of produced ammonia

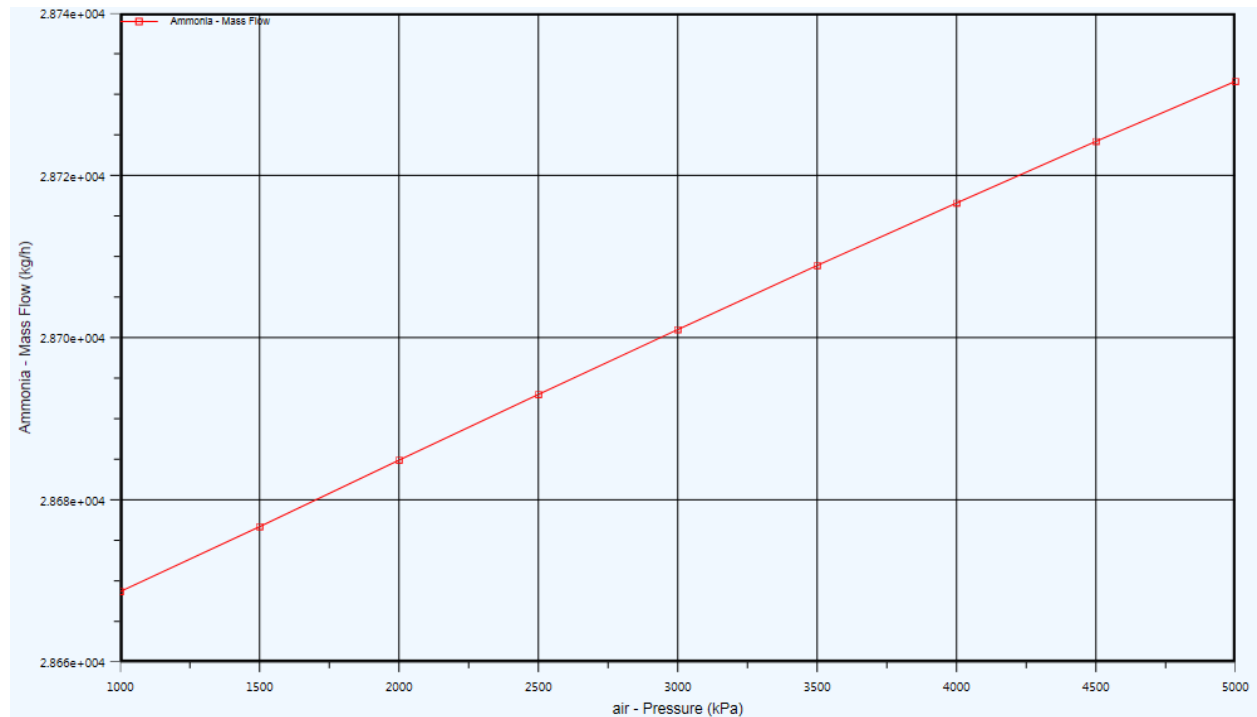


Figure 13: pressure of feed of air vs. Mass flow rate of produced ammonia

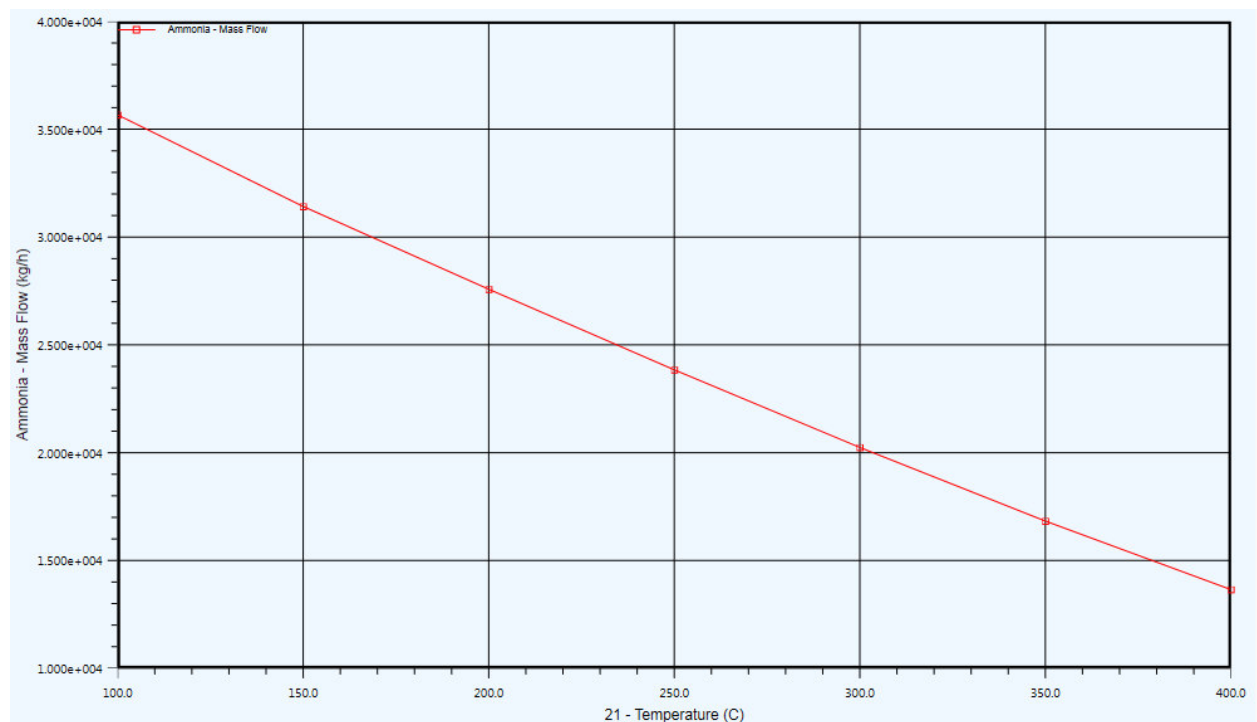


Figure 14: temperature of feed of nitrogen and hydrogen vs. Mass flow rate of produced ammonia

4. Conclusion

Ammonia production is an essential chemical process because of its applications. In this paper, the produced information in light of the recreation performed in HYSYS. This information can enable us to comprehend the procedure in various circumstances in mechanical practice. By changing the distinctive parameters in this recreation condition, the impacts of these parameters on ammonia production are watched and the outcomes are appeared in graphical shape. Utilizing the plots, the ideal conditions for ammonia production can be effortlessly discovered.

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