USING ASPEN HYSYS SOFTWARE FOR THE SIMULATION OF AMMONIA PRODUCTION PLANT

[1] **Pr.Dr.Nabil Abdel El Moneim,** [2] **Pr.Dr.Ibrahim Ismail,** [3] **Nasser. M.M**
[1] Cairo University, Faculty of Engineering [2] Cairo University, Faculty of Engineering [3] 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 saves a lot of time and also a lot of money. Today, there are many numbers 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 industries 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 changing different processing parameters in this simulation environment, the impact of these parameters in ammonia production rate is watched.

Keywords: Ammonia, Simulation, Aspen Hysys

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.

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.

4.1 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) CO_2 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^{0}C in the presence of a nickel catalyst where methane is changed over to hydrogen, carbon dioxide and little amounts of carbon monoxide.

$$CH_4 + 2H_2O \rightarrow CO_2 + 4H_2 \quad\ldots\ldots (1)$$

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad\ldots\ldots (2)$$

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

$$2CH_4 + O_2 \rightarrow 2CO + 4H_2 \quad\ldots\ldots (3)$$

$$CH_4 + O_2 \rightarrow CO_2 + 2H_2 \ldots\ldots (4)$$

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^{0}C and likewise carbon monoxide is expelled and changed over to carbon dioxide at low temperature move change (325^{o}C).

$$CO + H_2O \rightarrow CO_2 + H_2 \ldots\ldots (5)$$

2.1.4 Ammonia Production:

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

$$N_2+3H_2 \rightarrow 2NH_3 \ldots\ldots (6)$$

2.2 Software:

The software used in the simulation of ammonia plant design is Aspen Hysys (v.8.8) with steady state mode.

2.3 Simulation of the process:

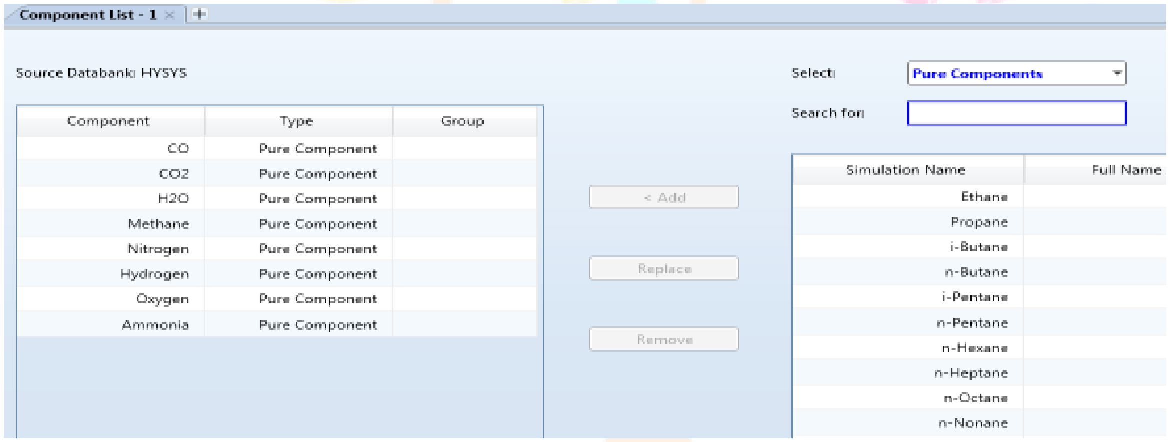
The main steps for ammonia process simulation by using aspen hysys are the following:

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 (14) 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 CH_4, H_2O, CO, CO_2, N_2, H_2, O_2 ignoring sulfur content as the components for the ammonia production. Figure (01) demonstrates the used component list in aspen hysys programming.



Component List - 1

Source Databank: HYSYS

Component	Type	Group
CO	Pure Component	
CO2	Pure Component	
H2O	Pure Component	
Methane	Pure Component	
Nitrogen	Pure Component	
Hydrogen	Pure Component	
Oxygen	Pure Component	
Ammonia	Pure Component	

Select: Pure Components

Search for:

Simulation Name	Full Name
Ethane	
Propane	
i-Butane	
n-Butane	
i-Pentane	
n-Pentane	
n-Hexane	
n-Heptane	
n-Octane	
n-Nonane	

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.

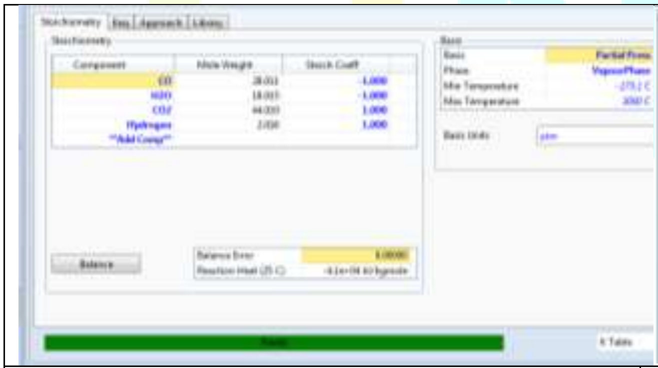


Figure (02) design the reaction (set-1) of HTSC & LTSC reactor.

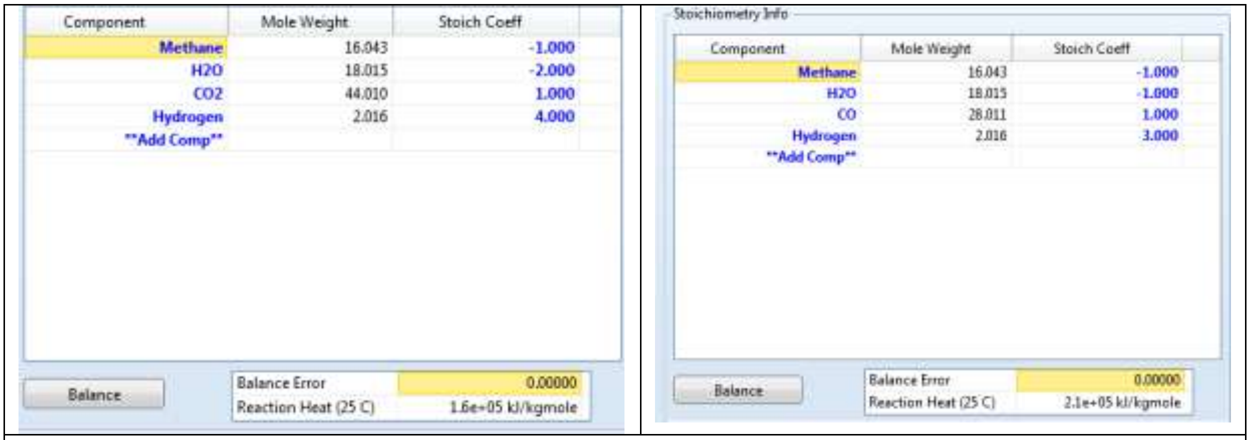
Stoichiometry Info

Component	Mole Weight	Stoich Coeff
CO	28.011	-1.000
Hydrogen	2.016	-3.000
Methane	16.043	1.000
H2O	18.015	1.000
Add Comp		

Balance Error: 0.00000

Reaction Heat (25 C): -2.1e+05 kJ/kgmole

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



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		

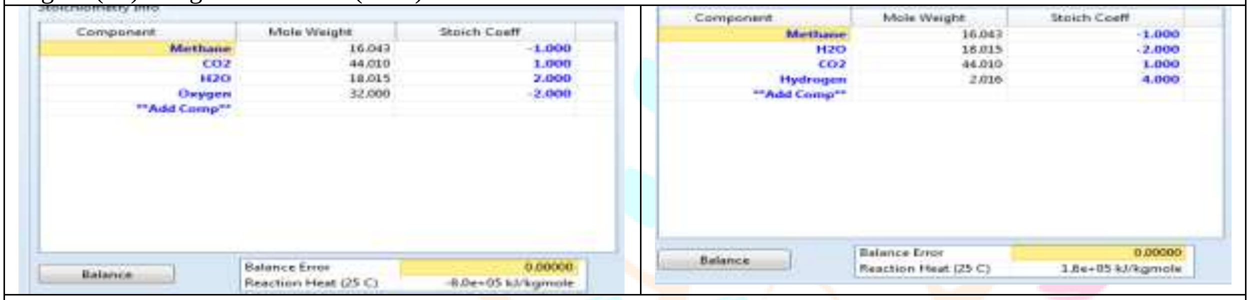
Balance Error 0.00000
Reaction Heat (25 C) 1.6e+05 kJ/kgmole

Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-1.000
CO	28.011	1.000
Hydrogen	2.016	3.000
Add Comp		

Balance Error 0.00000
Reaction Heat (25 C) 2.1e+05 kJ/kgmole

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



Stoichiometry Info

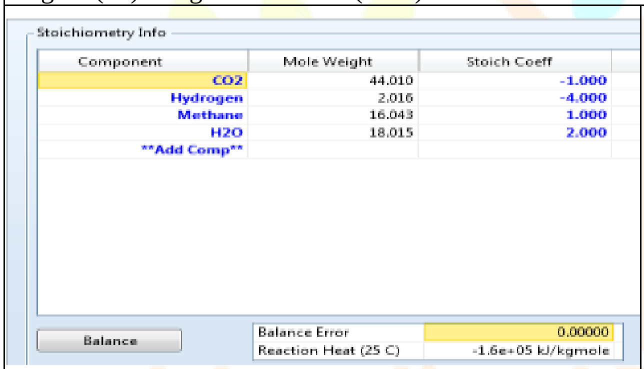
Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
CO2	44.010	1.000
H2O	18.015	2.000
Oxygen	32.000	-2.000
Add Comp		

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

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) 1.8e+05 kJ/kgmole

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

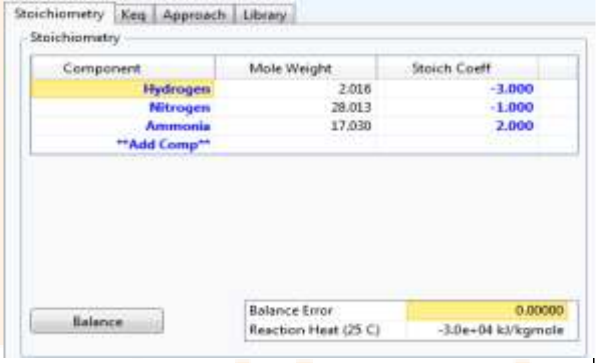


Stoichiometry Info

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		

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

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



Stoichiometry

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) -3.0e+04 kJ/kgmole

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 (1).

Table (1) the basic streams conditions for the simulation

Stream	Temperature (^oC)	Pressure (Kpa)	Component mole fraction						
			Ch4	H_2O	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.

3.1Temperature of natural gas:

From the figure (08), it is clear that there is an influence of the temperature of the natural gas on ammonia production rate where an increase of the temperature of natural gas causes a decrease in the ammonia production rate. This is due to this reason, the increase of the temperature of the natural gas causes methane cracking that is lead to influence on the steam to carbon ratio in the first reformer and according to le Chatelier's principle the reaction of steam reformation of methane is endothermic reaction so increasing temperature cause the reaction to go to the direction of the production of hydrogen and decreasing the used amount of steam and methane. This decrease causes the decrease in the efficiency of high and low shift conversion that used steam to convert carbon monoxide to carbon dioxide in addition to increase the energy demand and steam demand that is used in secondary reformer and in other equipment.

3. 2 Temperature of steam:

From the the figure (9), the influence of temperature of steam on ammonia production rate is very clear in three intervals as from 200-250 ^{0}K the increase of the temperature cause increase of the ammonia production rate & from 250-300 ^{0}K the maximum ammonia production rate is obtained & from higher than 300 ^{0}K the increase of temperature cause decrease of ammonia production rate so the optimum operating temperature of steam is from 250-300 ^{0}K.

3. 3 Pressure of steam:

From the figure (10), it is observed that the increase of steam pressure causes an increase of the ammonia production rate. The reason for this is according to le Chatelier's principle the reaction of steam reformation of methane is endothermic reaction so increasing pressure cause the reaction to go to the direction of low number of moles that is the direction of the production of hydrogen and decreasing the used amount of steam and methane.

3.4 Temperature of air:

From the figure (11), the influence of the temperature of air is clear where the temperature of air is inversely proportional to the ammonia production rate. This is due to le Chatelier's principle the reaction of air with the methane is exothermic reaction so increasing temperature cause the reaction to go to the direction of the backward reaction(used amount of air and methane) not the forward reaction (production of nitrogen).

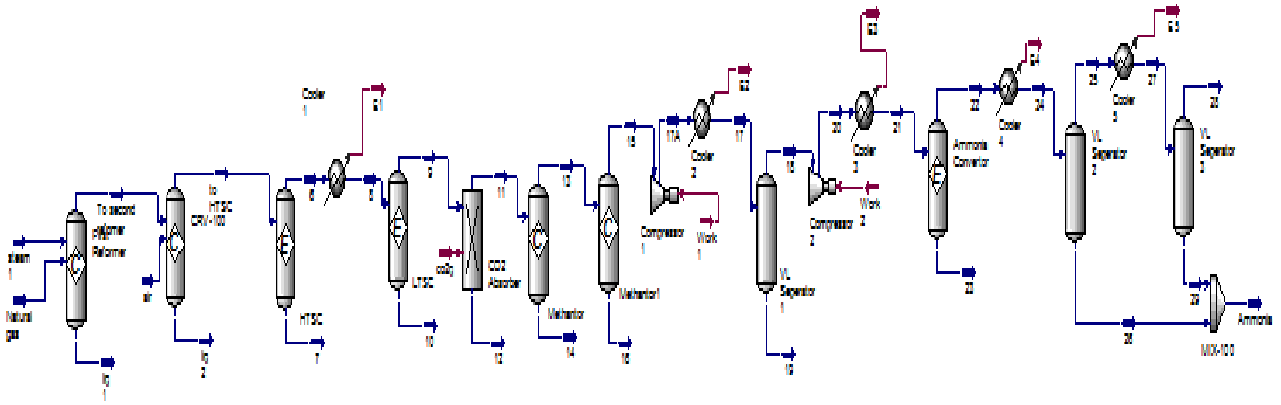
3.6 Pressure of air:

From the figure (12), it is observed that the increase of the pressure of air cause increase on the production rate. The reason for this is according to le Chatelier's principle the reaction of air with the methane is exothermic reaction and increasing pressure cause the reaction to go to the direction of low number of moles that is the direction of the production of nitrogen and decreasing the used amount of air and methane thus the increase in the pressure of feed air cause an increase in the amount of nitrogen that lead to increase the production rate of ammonia.

3.7 temperature of the feed (hydrogen & nitrogen)

From the figure (13), it is clear that the increase of the feed temperature causes decreases in the ammonia production rate. This is due to le Chatelier's principle the reaction between hydrogen and nitrogen is exothermic reaction so increasing temperature causes the reaction to go to the direction of backward (direction of hydrogen and nitrogen) so decreasing temperature cause an increase in the ammonia production rate.

Figure (14) Hysys Process Flow diagram of ammonia synthesis



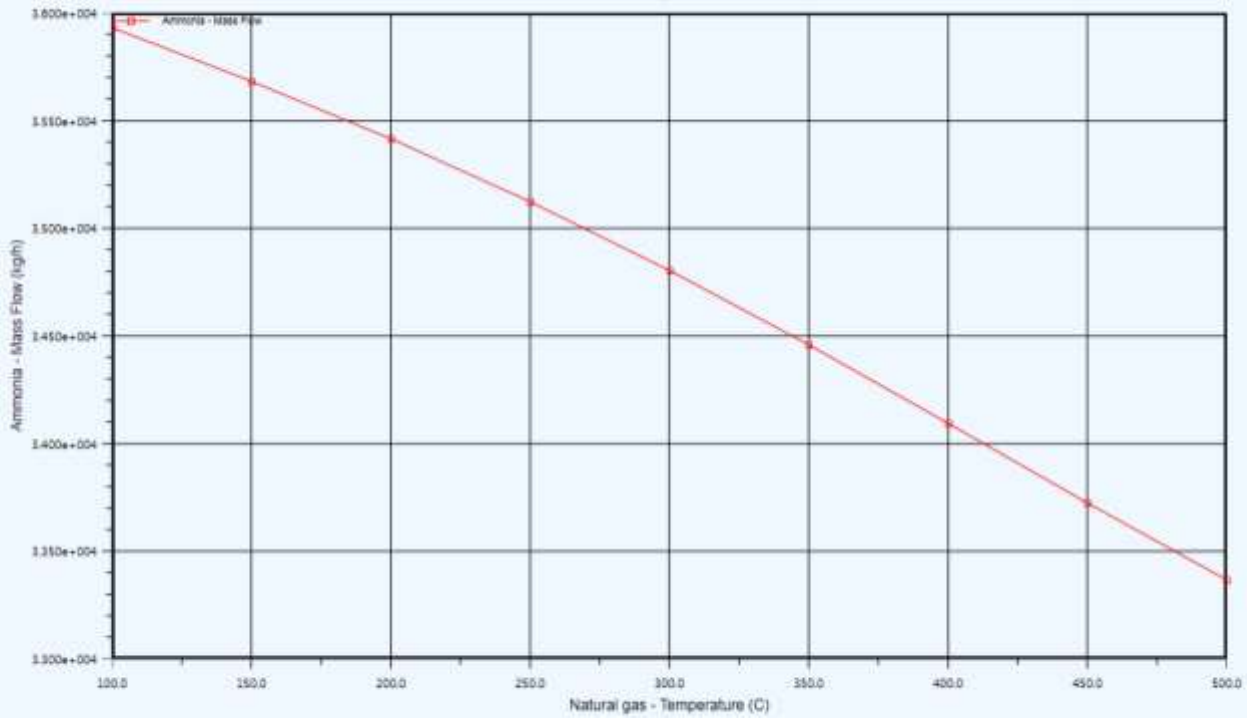


Figure 08: temperature of natural gas vs. Mass flow rate of ammonia

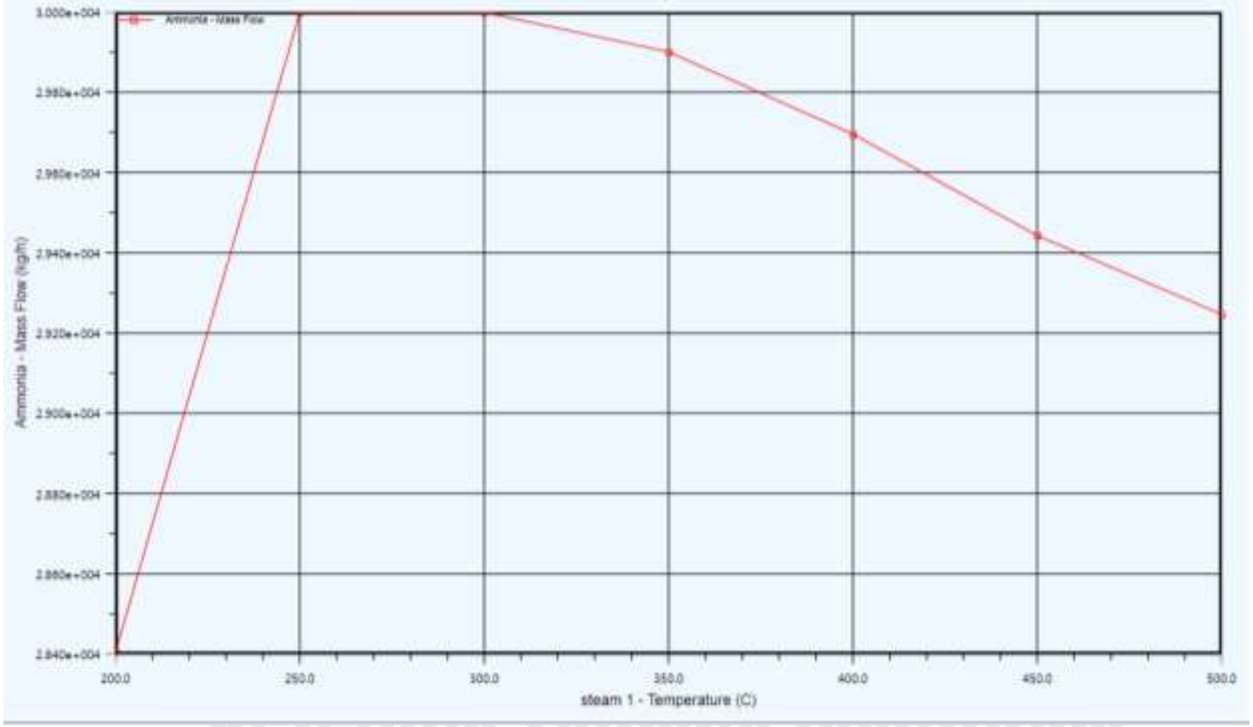


Figure 9: temperature of steam vs. Mass flow rate of produced ammonia.

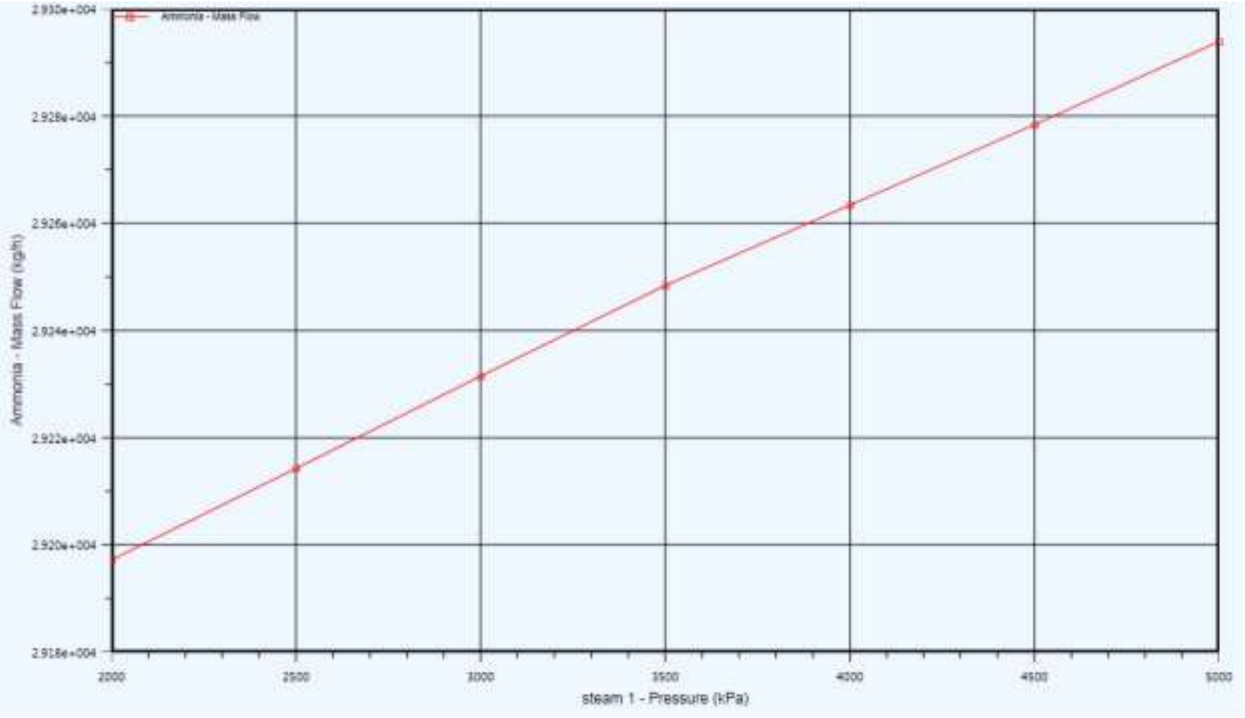


Figure 10: pressure of steam vs. Mass flow rate of produced ammonia.

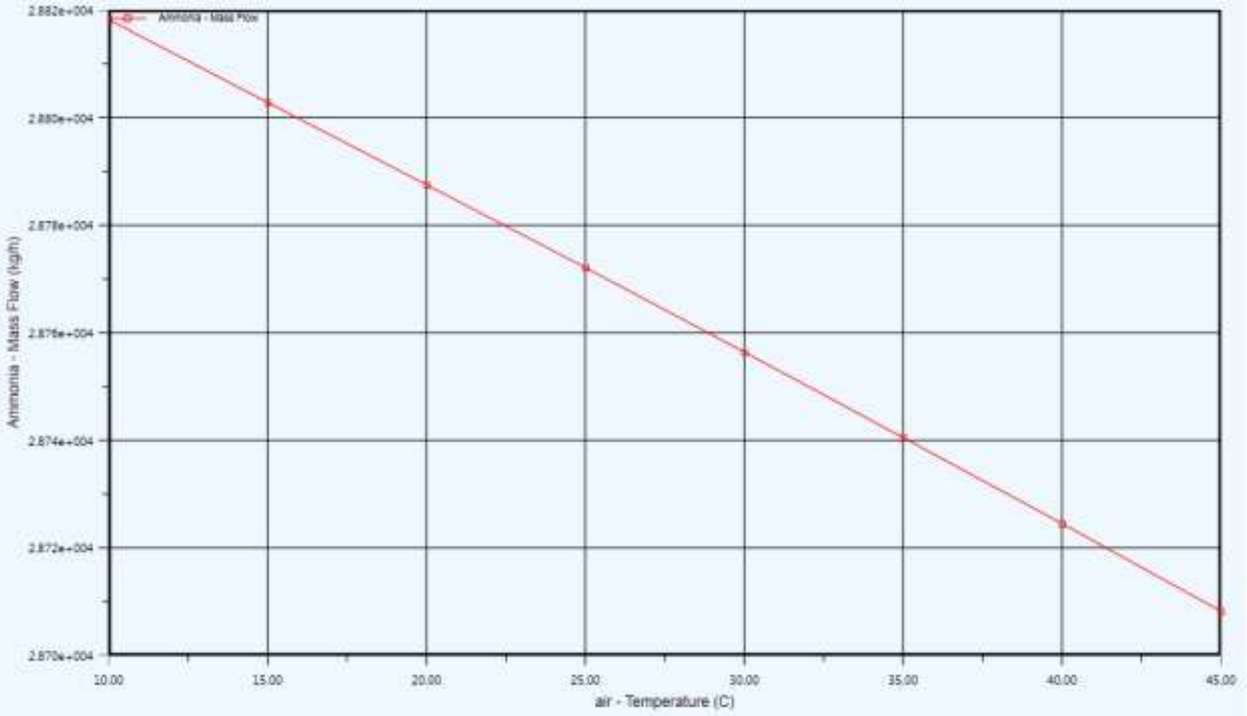


Figure 11: Temperature of feed of air vs. Mass flow rate of produced ammonia

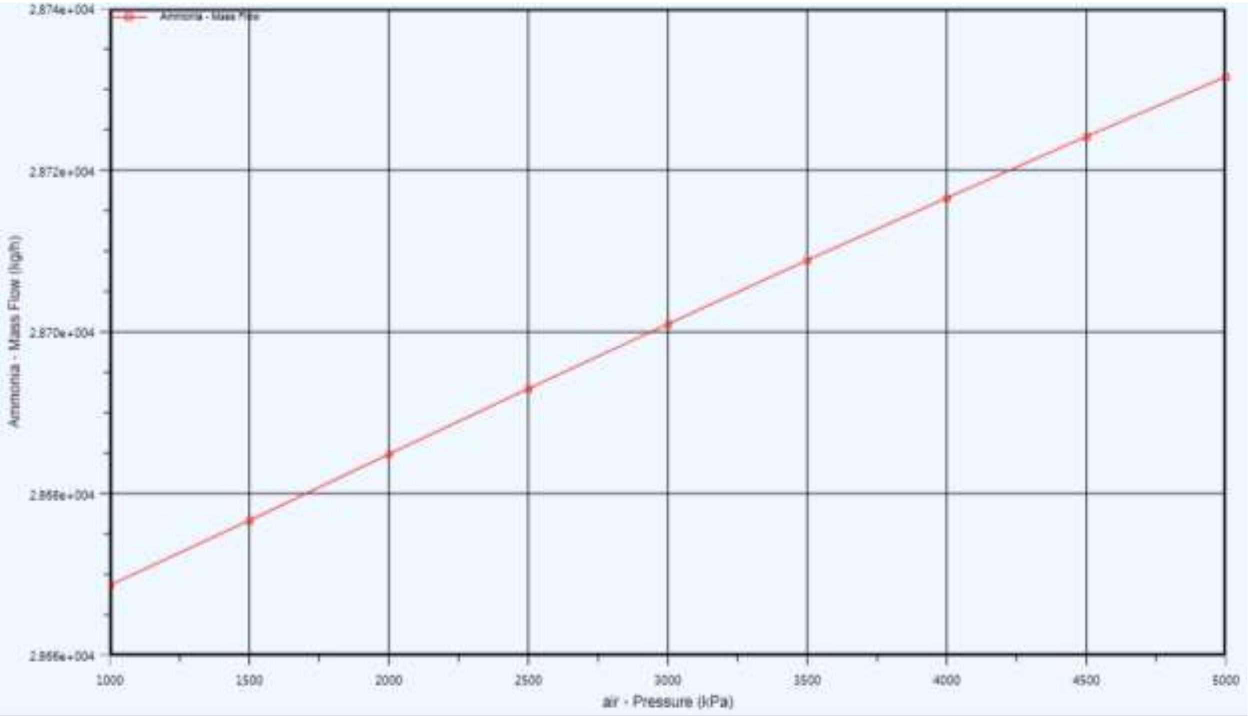


Figure 12: pressure of feed of air vs. Mass flow rate of produced ammonia

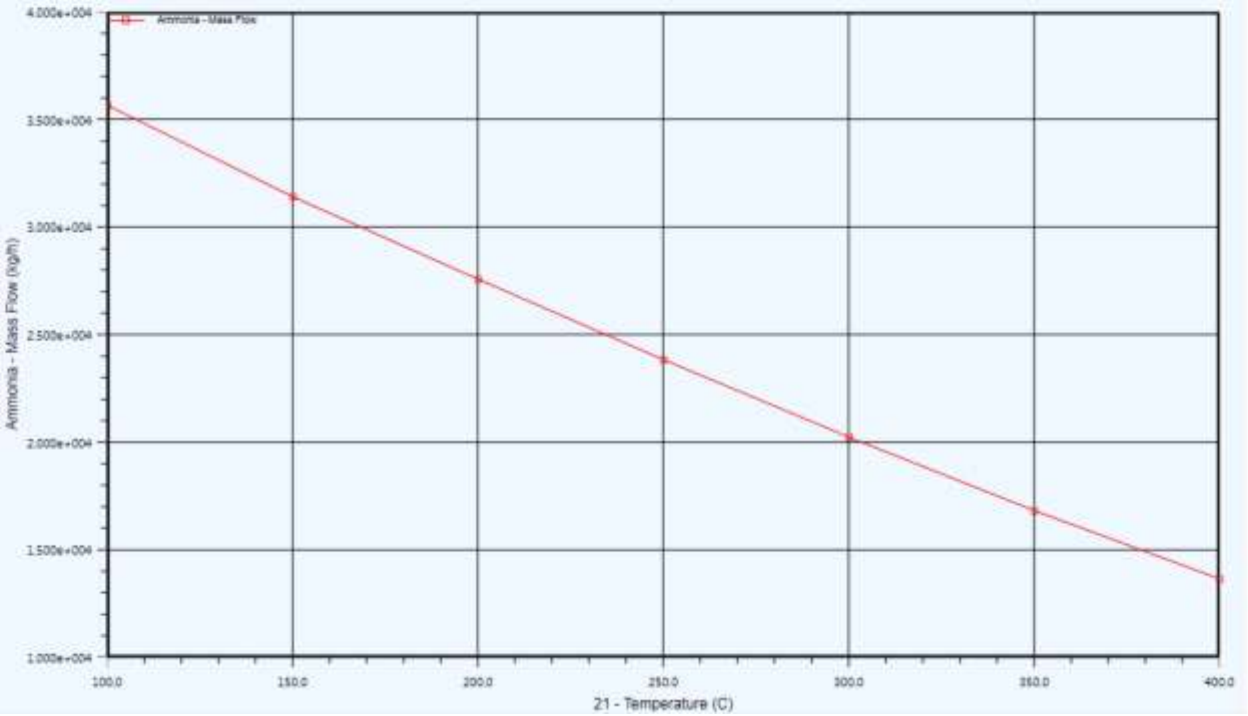


Figure 13: temperature of feed of nitrogen and hydrogen vs. Mass flow rate of produced ammonia

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 different processing 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.

REFERENCES:

[1] Amin, M. R., Sharear, S., Siddique, N., & Islam, S. Simulation of Ammonia Synthesis. American Journal of Chemical Engineering, (2013)1(3), 59-64.

[2] Appl, M. Ammonia. Ullmann's encyclopedia of industrial chemistry (2006).

[3] Biegler, L. T. Process flow sheet optimization: recent results and future directions (1987).

[4] Biegler, L. T., Grossmann, I. E., & Westerberg, A. W. Systematic methods for chemical process design (1997).

[5] Bland. Optimization of an ammonia synthesis loop (2015).

[6] Erisman, J. W., Sutton, M. A., Galloway, J., Klimont, Z., & Winiwarter, W. (2008). How a century of ammonia synthesis changed the world. Nature Geoscience, 1(10), 636.

[7] Gaines, L. D., & Gaddy, J. L. Process optimization by flow sheet simulation. Industrial & Engineering Chemistry Process Design and Development, (1976) 15(1), 206-211.

[8] Hamid, M. K. A. (2007). HYSYS: An Introduction to Chemical Engineering Simulation. Apostila de Hamid.

[9] HYSYS, A. (2013). Version 8.0. Aspen Technology Inc.

[10] Lawrence, S. A. (2004). Amines: synthesis, properties and applications. Cambridge University Press.

[11] Schlögl, R. (2003). Catalytic Synthesis of Ammonia—A “Never-Ending Story”?. Angewandte Chemie International Edition, 42(18), 2004-2008.

[12] Sotoft, L. F., Pryds, M. B., Nielsen, A. K., & Norddahl, B. Process Simulation of Ammonia Recovery from Biogas Digestate by Air Stripping with Reduced Chemical Consumption. In Computer Aided Chemical Engineering (2015) (Vol. 37, pp. 2465-2470). Elsevier.