Optimization of Operating Conditions for Enhanced Efficiency in Green Ammonia Production toward Sustainable Fertilizer Applications

Balqis Azzahra, Cornelley Kadja Pala*, Nayla Amira Andaristi, Ruqoya Akmalia, Yuliana Sinta Rizka Hapsari

Department of Chemical Engineering, Faculty of Engineering, Universitas Diponegoro, Semarang, Indonesia.

Abstract

This study investigates the enhancement of reaction efficiency in green ammonia production through the optimization of operating conditions using Aspen HYSYS simulation. Conventional ammonia synthesis is limited by its high energy demand, driven largely by extreme operating pressures and temperatures as well as the substantial load on compressors. To address these constraints, the process was modified by lowering the operating temperature in the main heating unit (Q-101) and adjusting compressor pressure and recycle streams, thereby shifting the reaction equilibrium toward product formation while reducing overall energy requirements. Simulation results reveal that decreasing the temperature from 482.5 °C to 368.9 °C significantly increased the molar flow rates of nitrogen, hydrogen, and particularly ammonia, which reached 185.5 kmol/h. This outcome confirms that lower temperatures in an exothermic reaction enhance conversion in accordance with Le Chatelier's principle. Furthermore, reducing the heat generated during compression lessens the demand on intercoolers and cooling units, improving overall thermal efficiency. The integration of multistage compressors and the recovery of waste heat provide additional gains in energy efficiency. Collectively, these findings demonstrate that relatively simple adjustments to operating parameters can substantially increase ammonia yield, lower energy consumption, and contribute meaningfully to process sustainability, reinforcing the potential of green ammonia as a more efficient and environmentally responsible pathway for low-carbon fertilizer production.
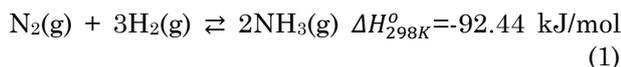
1. Introduction

Ammonia is a chemical compound consisting of one nitrogen (N) atom and three hydrogen (H) atoms. It is a colorless gas with a sharp, characteristic odor. In its pure form, ammonia is known as ammonia gas or anhydrous ammonia, as it contains no water. This gas can be readily liquefied through compression, and it exhibits high solubility in water. When dissolved, it forms liquid ammonia or an aqueous ammonia solution. In aqueous environments, a significant portion of ammonia molecules convert into ammonium ions (NH_4^+), charged species generated through electron transfer processes. Unlike gaseous ammonia, which has a pungent odor, ammonium ions are odorless and do not exist in the gaseous phase. Ammonia and ammonium can interconvert depending on environmental conditions. In aquatic systems such as wells, rivers, and lakes, as well as in moist soils, ammonium is typically the dominant species [1]. Ammonia also possesses distinct physical properties, including a boiling point of –33.5 °C, a freezing point of –77.7 °C, and a critical temperature of 133 °C [2]. The chemical reaction responsible for the formation of ammonia is as follows [3]:

* Corresponding Author.
Email: cornelleykdjp@gmail.com (C.K. Pala)

$$N_2(g) + 3H_2(g) \rightleftarrows 2NH_3(g) \ \Delta H^o_{298K} = -92.44 \ \text{kJ/mol} \tag{1}$$

Ammonia production is constrained by three primary factors: catalytic reaction resistance, ammonia separation via condensation, and the recycling of unreacted gases. Ongoing research explores wind-powered fertilizer production technologies as sustainable alternatives to fossil fuels. To analyze ammonia synthesis in small-scale Haber–Bosch units and identify optimal operating conditions, the process is commonly simplified into three stages: reaction, separation, and recycling. This modeling framework effectively captures the performance of each unit and provides valuable insights into the characteristics of different process zones. Laboratory kinetic studies and reaction rate linearization indicate that the chemical reaction stage is the principal limiting factor in overall ammonia production [4].

Despite remaining the predominant method of ammonia production, the Haber–Bosch process is associated with several critical limitations. The reaction itself proceeds at a relatively slow rate and requires extremely high temperatures and pressures, consuming nearly 1% of global energy while contributing substantially to greenhouse gas emissions. Moreover, the hydrogen feedstock is typically obtained through steam methane reforming or coal gasification, processes that collectively release over 420 million tons of CO_2 annually, thereby exacerbating environmental concerns. The conversion efficiency of the process is also inherently low—approximately 15–20% per single pass, necessitating extensive gas recycling to achieve overall conversions approaching 97% [5]. Consequently, the conventional Haber–Bosch process is both environmentally unsustainable and inefficient in terms of energy utilization.

Accordingly, research on the optimization of operating conditions to enhance the efficiency of green ammonia synthesis is of paramount importance, particularly in advancing the sustainable development of green fertilizers.
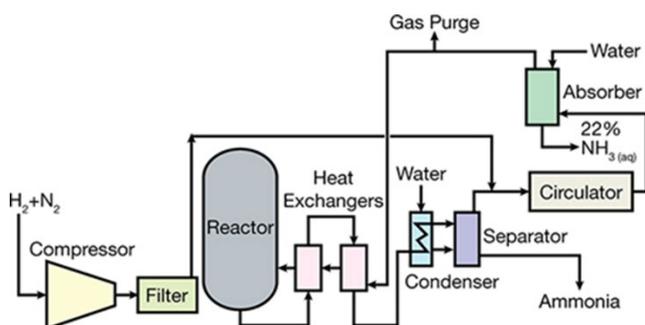
Adjustments to operating parameters have been demonstrated to reduce compression demands, improve reaction conversion, and lower overall energy consumption. In this context, the present study is directed toward the systematic analysis and optimization of operating conditions in ammonia synthesis, with the objective of improving reaction efficiency and thereby promoting a more environmentally sustainable and industrially viable pathway for future fertilizer production.

2. Methods

2.1 Basic Process Flow Diagram

Figure 1 presents the Basic Process Flow Diagram for green ammonia production, which serves as the basis for the process simulation undertaken in this study. The production pathway has not yet achieved complete conversion, as residual ammonia remains in the exhaust stream. For this simulation, the Peng–Robinson property package was employed. This equation of state was selected due to its proven suitability for modeling gas–liquid, liquid–liquid, and vapor–liquid equilibria, as well as multicomponent systems containing hydrocarbons. Accordingly, the Peng–Robinson model is considered an appropriate and reliable framework for representing the thermodynamic behavior of green ammonia production [6].

2.2 Modification Method to Improve the Process

Optimization can be achieved through modifying the key operation of the process. Reactor inlet temperature and recycle stream pressure were selected to be modified. The objective function of the optimization is to maximize the molar flow rate of ammonia at the reactor outlet, which directly reflects the reaction conversion. Elevated pressure shifts the equilibrium toward product formation, as the total number of gas moles in the products is lower than in the reactants. Temperature regulation, on the other hand, ensures that the reaction proceeds at its optimum temperature, thereby maintaining a balance between reaction rate and conversion efficiency. Collectively, these adjustments enable more effective control of the reaction pathway and improve overall process performance [8].

The optimization procedure was performed by reducing the reactor inlet temperature from 482.5 °C to 368.9 °C through adjustment of the heat exchanger (Q-101). Since ammonia synthesis is an exothermic reaction, lowering the operating temperature shifts the equilibrium toward product formation in accordance with Le Chatelier's principle, thereby increasing conversion. Pressure levels in the compressor and

Figure 1. Basic process flow diagram (unmodified) [7].

recycle streams were subsequently adjusted to maintain pressure compatibility and stable reactor operation. The recycle stream pressure is elevated by means of a compressor prior to re-entering the mixer, thereby ensuring consistency with the pressure of the other process streams [9].

The analysis was conducted by comparing the number of moles of NH₃ produced with the number of moles of reactants introduced into the system. Reaction efficiency serves as a key parameter for assessing the extent to which a chemical reaction converts reactants into products in accordance with the desired stoichiometry. Within this framework, reaction efficiency is employed to evaluate the effectiveness of reactant conversion in the reactor, thereby quantifying the proportion of reactants that undergo transformation. The expression for reaction efficiency utilized in this study is given as:

$$Conversion\,(\%)= \frac{Moles\ of\ NH_3\ formed}{Moles\ total\ of\ N_2\ and\ H_2\ fed} \times 100\% \qquad (2)$$

3. Results and Discussion

One of the most effective strategies for enhancing energy efficiency in the Haber-Bosch ammonia synthesis process is to reduce compressor workload, thereby directly lowering the energy demand of both compressors and downstream cooling systems [4]. The Haber-Bosch process accounts for approximately 1–2% of global annual energy consumption, primarily due to its high operating temperatures (573–873 K) and pressures (100–350 bar), as well as its dependence on hydrogen derived from natural gas as a feedstock [10]. Compressors consume substantial electrical energy to pressurize the synthesis gas (a mixture of hydrogen and nitrogen), and the associated temperature rise increases the demand for intercoolers and heat exchangers to dissipate the heat generated during compression [11]. In this study, process simulations were performed using Aspen HYSYS V11 to assess how operating conditions influence overall energy consumption and reactor performance. The primary objective is to optimize product conversion and improve mass efficiency by incorporating recycle streams into the production process.

Based on ammonia synthesis simulation data obtained using Aspen HYSYS V10 [12], the energy flow rates summarized in Table 1 demonstrate that the applied strategy significantly increased ammonia yield. Prior to modification, the process produced 7.058 kg/h of ammonia, whereas after modification the yield rose to 8.969 kg/h, representing a 27.08% improvement. This increase in output highlights the influence of several critical factors within the reaction process. The findings further indicate that lowering the operating temperature in K-01 (stream Q-101) directly impacts the pressure in subsequent operating stages, thereby altering overall process performance.

Figure 1 shows that under the baseline operating conditions, ammonia synthesis begins with the mixing of nitrogen and hydrogen at 25 °C and 101.3 kPa. The stream then passes through heat exchangers and compressors, raising the temperature to 438 °C and the pressure to 2.553×10^4 kPa before entering the reactor. The resulting ammonia product subsequently experiences a reduction in temperature and pressure to –35.5 °C and 101.3 kPa. Following modification of the operating conditions—specifically, lowering the temperature in stream Q-101 to 368.9 °C while maintaining the pressure at 101.3 kPa—the stream again passes through the heat exchangers and compressors before entering the reactor, yielding ammonia at –34.9 °C and 101.3 kPa. This adjustment demonstrates that reducing the operating temperature directly limits heat generation, thereby decreasing the cooling energy demand of the system, particularly in the intercooler and condenser units. The outcomes of this modification are presented in Figure 2.

The ammonia synthesis process was modified by lowering the operating temperature in K-01 (Q-101), reducing it by 113.7 °C from 482.5 °C to 368.9 °C. This adjustment not only altered the final temperature of the ammonia but also affected key process parameters, including vapor fraction, pressure, molar flow, mass flow, liquid volume flow, and heat flow of nitrogen, hydrogen, and ammonia. The operating condition data for hydrogen and nitrogen as feed inputs, along with ammonia as the product output, are summarized in Tables 1 and 2. The data
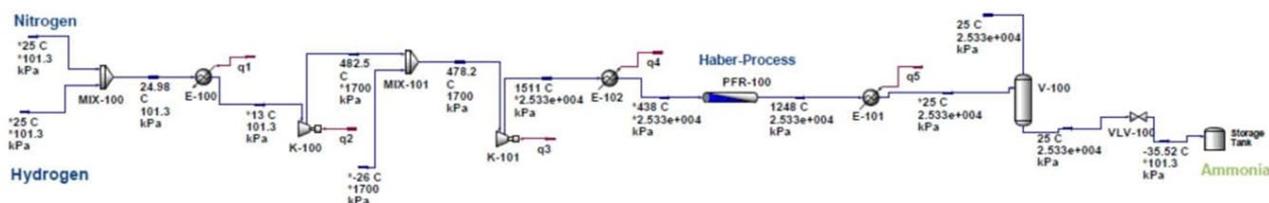

Figure 2. Process flowchart of green ammonia synthesis on Aspen HYSYS V10 before modification

presented in Tables 1 and 2 indicate that, following modification, the molar flow rates of nitrogen and hydrogen increased, accompanied by a substantial rise in the molar flow rate of ammonia, reaching 185.5 kmol/h with a corresponding mass of 3307 kg/h. These results confirm that lowering the operating temperature effectively enhances both ammonia conversion and overall production. Given that ammonia synthesis is an exothermic reaction, a reduction in temperature shifts the equilibrium toward ammonia formation in accordance with Le Chatelier's principle, while elevated pressure further improves conversion efficiency [4, 13, 14]. The simulation outcomes are also consistent with reported literature, which demonstrates that at 200 bar and an inlet temperature of 400 °C, ammonia concentrations can exceed 20% per pass [9].

Energy integration within compressors and cooling stages is a critical factor in enhancing overall process efficiency. The application of multistage compressors with intercooling offers an optimal balance between energy savings and capital investment, with ideal operating pressures typically ranging from 75 to 150 bar [15]. Furthermore, optimizing the interstage pressure ratio can significantly reduce compressor work by aligning with the specific process configuration [16]. In addition, the substantial waste heat generated from the synthesis reaction, amounting to 2.7 GJ per ton of NH_3, together with heat from the electrolysis process, can be harnessed to produce high-pressure steam for driving compressor turbines [13]. Effective utilization of this waste heat has been demonstrated to markedly improve the overall energy efficiency of the system.

Table 1. Datasheets for input and output streams before modification.

Parameter	Unit	Nitrogen	Hydrogen	Ammonia
Vapour fraction		1	1	0
Temperature	°C	25	25	-35.52
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmole/h	249.2	646.1	-
Mass flow	kg/h	7000	1400	-
Liquid volume flow	m³/h	8.632	-1944	-
Heat flow	kJ/h	18.62	-4.138E5	-

Table 2. Datasheets for input and output streams after modification.

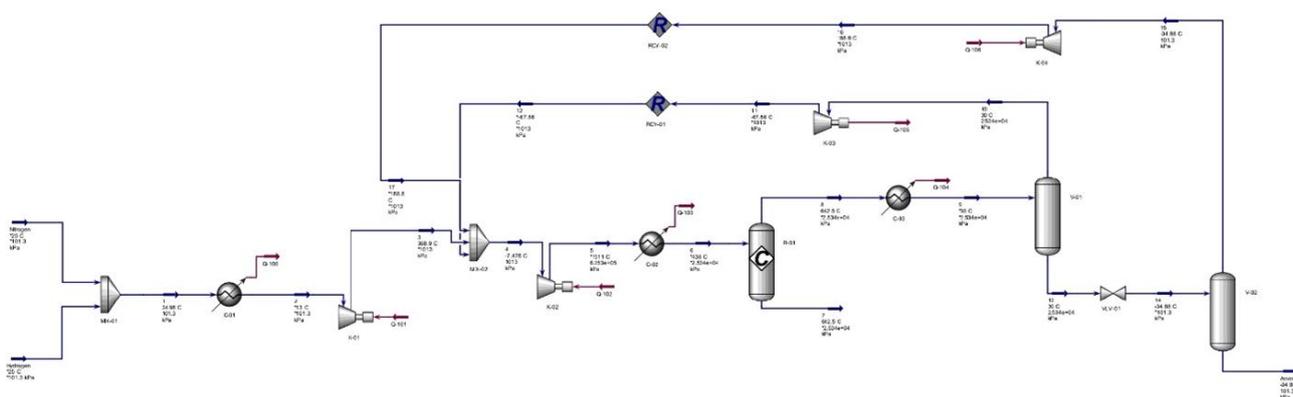| Parameter	Unit	Nitrogen	Hydrogen	Ammonia
Vapour fraction		1	1	0
Temperature	°C	25	25	-34.88
Pressure	kPa	101.3	101.3	101.3
Molar flow	kgmole/h	285.6	793.7	185.5
Mass flow	kg/h	8000	1600	3307
Liquid volume flow	m³/h	9.921	22.90	5.238
Heat flow	kJ/h	-2219	-86.47	-8.114E6

Figure 3. Process simulation of green ammonia synthesis on Aspen HYSYS V11 after modification.

A modified process was implemented to increase the molar flow rate of ammonia at the reactor outlet. The optimization approach was carried out by lowering the temperature at the K-101 (stream-101) operating conditions and adjusting the compressor pressure to maintain reaction stability. The reactor inlet temperature was used as an independent variable in the modification of green ammonia production, with the temperature being lowered from 482 °C to 368.9 °C. In accordance with Le Chatelier's principle, the temperature reduction under operating conditions was carried out to shift the reaction equilibrium towards NH_3 formation.

From both environmental and economic perspectives, optimizing operating conditions in green ammonia production is highly impactful. Conventional ammonia synthesis via the Haber–Bosch process accounts for approximately 1.2% of global carbon emissions, releasing more than 400 million tons of CO_2 annually [17, 18]. Transitioning from hydrogen produced through steam methane reforming to electrolytic hydrogen generated from renewable energy sources could reduce emissions by up to 78% while improving process energy efficiency by nearly 50% [13]. Furthermore, small-scale distributed e-ammonia production provides operational flexibility and represents a key pathway in advancing the transition toward a carbon-neutral industry [3].

4. Conclusion

This study confirms that optimizing operating parameters, particularly by lowering reactor inlet temperature and adjusting compressor pressures, can markedly improve the efficiency of green ammonia synthesis. Such modifications shift the reaction equilibrium toward greater ammonia formation while simultaneously reducing compression energy demand, thereby advancing the field beyond the inherent limitations of the conventional Haber–Bosch process. The incorporation of multistage compressors and effective waste heat recovery further strengthens the case for enhanced thermal efficiency and reduced carbon emissions, positioning green ammonia as a practical and sustainable alternative for low-carbon fertilizer production. Importantly, the findings demonstrate that relatively straightforward process adjustments can deliver significant gains in conversion efficiency and energy utilization, contributing to the broader pursuit of carbon-neutral chemical manufacturing. Future work should prioritize pilot-scale validation of these simulation results, investigate advanced catalyst systems capable of operating under milder conditions, and integrate renewable hydrogen sources to maximize environmental benefits. In parallel, ongoing developments in distributed e-ammonia production and membrane reactor technologies offer promising avenues to extend and diversify the applicability of this optimization framework.

References

[1] Roney, N., Llados, F., Little, S.S., Knaebel, D.B. (2004). Toxicological Profile for Ammonia. In N. Roney, F. Llados, S. S. Little, & D. B. Knaebel (Eds.), Federal Register (Issue September). U.S. Departement of Health and Human Service Public Health Service Agency for Toxic Substances and Disease Registry. https://www.atsdr.cdc.gov/toxprofiles/tp126.pdf.

[2] Kartika, D., Wahyuningsih, P. (2019). Analisis Kandungan Amoniak dalam Limbah Outlet KPPL PT. Pupuk Iskandar Muda (PT. PIM) Lhokseumawe. *Jurnal Kimia Sains dan Terapan*, 1(2), 6-10. https://ejurnalunsam.id/index.php/JQ/article/view/1692/1266.

[3] de la Hera, G., Ruiz-Gutiérrez, G., Viguri, J. R., Galán, B. (2024). Flexible green ammonia production plants: Small-Scale simulations based on energy aspects. *Environments*, 11(4), 71. DOI: 10.3390/environments11040071

[4] Reese, M., Marquart, C., Malmali, M., Wagner, K., Buchanan, E., McCormick, A., Cussler, E.L. (2016). Performance of a Small-Scale Haber Process. *Industrial & Engineering Chemistry Research*, 33, 3742-3750. DOI: 10.1021/acs.iecr.5b04909.

[5] Kou, Z., Shi, D., Yang, B., Li, Z., Zhang, Q., Lu, J., Zhang, T., Lei, L., Li, Y., Dai, L., Hou, Y., (2025). Efficient green synthesis of ammonia: from mechanistic understanding to reactor design for potential production. *Chemical Society Reviews*, 54, 10796-10844. DOI: 10.1039/d5cs00969c.

[6] Pelaquim, F.P., Bitencourt, R.G., Neto, A.M.B., Dalmolin, I.A.L., da Costa, M.C. (2022). Carbon dioxide solubility in Deep Eutectic Solvents: Modelling using Cubic Plus Association and Peng-Robinson equations of state. *Process Safety and Environmental Protection*, 163, 14 26. DOI: 10.1016/j.psep.2022.04.075.

[7] Pattabathula, V., Richardson, J. (2016). Introduction to ammonia production. *Chem. Eng. Prog*, 112(9), 69-75. https://www.aiche.org/sites/default/files/cep/20160969.pdf

[8] Mansourian, R., Mousavi, S.M., Rahimpour, M.R. (2024). Membrane reactors for ammonia synthesis/production. In *Progresses in Ammonia: Science, Technology and Membranes*, 111-130. DOI: 10.1016/B978-0-323-88502-7.00009-X.

[9] Tripodi, A., Compagnoni, M., Bahadori, E., Rossetti, I. (2018). Process simulation of ammonia synthesis over optimized Ru/C catalyst and multibed Fe + Ru configurations. *Journal of Industrial and Engineering Chemistry*. 66, 176-186. DOI: 10.1016/j.jiec.2018.05.027.

[10] Wang, T., Abild-Pedersen, F. (2021). Achieving industrial ammonia synthesis rates at near-ambient conditions through modified scaling relations on a confined dual site. *PNAS*, 118(30), 1-5. DOI: 10.1073/pnas.2106527118.

[11] Jiang, X., Liu, Y., Deng, Y., Wang, Z., Xu, R. (2023). Numerical analysis of a miniature multi-stage compressor at variable altitudes based on stages-in-series method. *Applied Thermal Engineering*, 219, 1359-4311. DOI: 10.1016/j.applthermaleng.2022.119563.

[12] Shaker, I., El-Bagoury, M., Yaser, S., Emad, H, Hamdy, O., Abouseada, N., Bassyouni, M., Aboelela, D. (2024). Process Simulation and Design of Green Ammonia Production Plant for Carbon Neutrality. *International Journal of Industry and Sustainable Development*, 5(1), 2682-3993. DOI: 10.21608/ijisd.2024.247887.1041.

[13] Smith, C., Hill, A.K., Torrente-Murciano, L. (2020). Current and future role of Haber–Bosch ammonia in a carbon-free energy landscape. *Energy & Environmental Science*, 13, 331-344. DOI: 10.1039/c9ee02873k.

[14] Palys, M.J., Wang, H., Zhang, Q., Daoutidis, P. (2021). Reneweable ammonia for sustainable energy and agriculture: vision and systems engineering opportunities. *Current Oppinion in Chemical Engineering*, 31, 100667. DOI: 10.1016/j.coche.2020.100667.

[15] Verleysen, K., Coppitters, D., Parente, A., De Paepe, W., Contino, F. (2020). How can power-to-ammonia be reboust? Optimization of an ammonia synthesis plant powered by a wind turbine considering operational uncertainties. *Fuel*, 266, 117049. DOI: 10.1016/j.fuel.2020.117049.

[16] Cheema, I.I., Krewer, U. (2018). Operating envelope of Haber-Bosch process design for power-to-ammonia. *RSC Advances*, 8, 34926-34936. DOI: 10.1039/C8RA06821F.

[17] D'Angelo, S.C., Cobo, S., Tulus, V., Nabera, A., Martin, A.J., Perez-Ramirez, J., Guillen-Gosalbez, G. (2021). Planetary Boundaries Analysis of Low-Carbon Ammonia Production Routes. *ACS Sustainable Chemistry & Engineering*, 9, 9740-9749. DOI: 10.1021/acssuschemeng.1c01915.

[18] Ghavam, S., Vahdati, M., Wilson, I.A., Strying, P. (2021). Sustainable Ammonia Production Processes. *Frontiers in Energy Research*, 9, 580808. DOI: 10.3389/fenrg.2021.580808