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Research Article

Improving Energy Efficiency in Ammonia Production from Hydrogen and Nitrogen Through Optimizing Operating Condition

Daffa Pratama Ramadhan, Fransiska Klarisa Teodora Hutasoit, Ghazy Arya Primaditya, Muhammad Verrel Aurielly*, Muhammad Yusuf Zachraey Muafi

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

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Abstract

As a key raw material in the fertilizer industry, global ammonia consumption showed a steady increase from 2010 to 2020, with an average annual growth rate of approximately 1.81%. The production of ammonia involves four primary stages: feed gas pre-treatment, syngas generation, syngas purification, and ammonia synthesis. The main feedstocks used in this process are natural gas, steam, and air. To accommodate the rising demand for ammonia, it is essential to implement a highly efficient production process that ensures a high conversion rate. One strategy to enhance efficiency involves reducing the operating pressure in the ammonia production process proves to be an effective strategy for enhancing overall energy efficiency. This adjustment lowers the compressor workload, which in turn reduces system temperatures and eases the demand on the cooling system. Importantly, the process maintains a gas-phase reaction environment and high conversion efficiency, indicating that energy savings are achieved without compromising reaction performance. The results confirm that pressure optimization lies within the thermodynamic and kinetic boundaries necessary for effective ammonia synthesis.

Keywords: Ammonia; Energy Efficiency; Process Design; Optimizing Operating Condition

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1. Introduction

Syngas is a type of fuel composed of a mixture of hydrogen (H_2), carbon monoxide (CO), and methane (CH_4) [1].It may also contain trace amounts of argon (Ar) and nitrogen (N_2), which are useful in the production of ammonia, ammonia, and Fischer-Tropsch liquids (FTLs). Ammonia possesses distinct physical properties, with a melting point of -57.5 °C and a boiling point of 37.7 °C . The gases involved in ammonia synthesis have unique characteristics; for instance, ammonia itself has a boiling point and melting point of -346 °F, and a critical temperature of -232.5 °F [2]. In comparison, hydrogen (H_2) has a melting point of -259.2 °C and a boiling point of -253 °C [3]. The production of syngas typically involves a partial oxidation process. The reaction is exothermic and requires minimal energy to initiate, but it necessitates effective heat removal from the catalyst to maintain optimal performance. When integrated with the Haber-Bosch (HB) process, which is the predominant method for industrial ammonia production, the process still demands a considerable amount of energy. Despite the exothermic nature of the ammonia synthesis reaction, a high energy input is needed.

Currently, ammonia synthesis accounts for approximately 1%–2% of global energy consumption. This substantial energy use is primarily attributed to the production of hydrogen, which is typically obtained through the

* Corresponding Author.
Email: verrelpro1st@students.undip.ac.id (M.V. Aurielly)

highly endothermic steam-methane reforming (SMR) process, operating at equilibrium temperatures between 800 °C and 1,000 °C. The chemical reaction involved is as follows [4]:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad \Delta H^o_{r,298K} = +206.1\ kJ/mol \quad (1)$$

In addition to reactant purification and compression, the resulting effluent gases are directed into a shift reactor where they are treated with excess steam at temperatures ranging from 350 °C to 550 °C. This process is aimed at converting carbon monoxide into additional hydrogen through the slightly exothermic water-gas shift (WGS) reaction, thereby enhancing hydrogen production efficiency:

$$CO + H_2O \rightarrow CO_2 + H_2 \quad \Delta H^o_{r,298K} = +41.2\ kJ.mol^{-1} \quad (3)$$

The Haber-Bosch process (HBP), commonly referred to as the Haber process, is one of the most widely used methods for synthesizing ammonia (NH_3). Ammonia produced through this process is recognized as one of the largest contributors to global energy consumption and CO_2 emissions. In industrial ammonia production facilities, hydrogen is typically derived from steam-methane reforming (SMR) followed by the water-gas shift (WGS) reaction, and then purified for use in high-pressure ammonia synthesis [2]. Extracting hydrogen from the reforming section improves the conversion of methane, which is otherwise restricted by thermodynamic limitations. Approximately 5%–14% of the protons introduced into the system are ultimately converted into ammonia . Given that the reaction is exothermic, effective cooling is essential to maintain stable reactor conditions .

Ammonia production can occur at atmospheric pressure by utilizing protons and electrons. The typical thermodynamic limitations of methane conversion at relatively low temperatures (550 °C–650 °C) can be overcome by removing hydrogen directly from the steam reforming section. Additionally, at these temperatures, methane is preferentially converted into carbon dioxide (CO_2) rather than carbon monoxide (CO), due to the predominance of the water-gas shift (WGS) reaction. This approach allows for maximum hydrogen production within a single unit, eliminating the necessity for a separate downstream shift reactor [5] .

The primary reaction responsible for producing ammonia occurs in the gas phase and is exothermic in nature. In this process, nitrogen gas (N_2) reacts with hydrogen gas (H_2) to form ammonia (NH_3) [7]. Following the synthesis within the reactor, the resulting mixture which still contains unreacted nitrogen and hydrogen along with the generated ammonia is subjected to cooling and separation. Historically, in 1898, Adolph Frank and Nikodem Caro discovered a method to fix nitrogen (N_2) using calcium carbide, forming calcium cyanamide, which could then be hydrolyzed to produce ammonia. However, due to the high energy demands of this process, scientific efforts later shifted toward developing methods with lower energy requirements.

The application of ML in chemical industries is starting to receive more attention in the literature. Machine learning algorithms were used for energy efficiency to optimize waste energy and reduce emission levels [8]. Machine learning models were also developed for the synthesis of Methyl Chloride (MC) from the methane chlorination process to predict reactor energy [9].

The production of ammonia relies on key raw materials such as natural gas, steam, and air. In an effort to enhance mass efficiency during the production process, a novel chemical looping system was developed for both hydrogen (H_2) and ammonia (NH_3) [6]. In our study, we introduced several modifications the combined analysis of simulation data, process configuration (PFD), and conceptual flowsheet supports the effectiveness of pressure reduction as an energy-saving measure in ammonia production [10].

2. Method

2.1 Basic Process Flow Diagram

The basic flow diagram depicted in Figure 1 forms the conceptual framework for the ammonia production process analyzed in this research. However, optimal ammonia yield is not achieved due to the loss of ammonia in the exhaust stream. To simulate the production process, the Peng-Robinson (PR) property package was utilized [8]. This thermodynamic model was selected because it is well-suited for systems involving hydrocarbons and provides reliable predictions for phase equilibria, including gas-liquid, gas-liquid-liquid, and multicomponent mixtures. As a result, the Peng-Robinson equation is considered highly appropriate for modeling the ammonia synthesis process [12].

2.2 Unmodified Method to Improve the Process

Prior to the implementation of the modification, the process did not incorporate an effective recycling system for the residual ammonia vapor produced after the separation stage (Figure 1) [6]. The unutilized vapor was either released or only partially redirected without adequate treatment or pressure adjustment. Furthermore, the system lacked a purge mechanism to remove inert or non-reactive components, leading to their accumulation over time. In addition, the absence of a compression unit resulted in a pressure mismatch between any recycled stream and the mixer inlet, thereby limiting the overall process efficiency and reducing the ammonia conversion rate

2.3 Modification Method to Improve the Process

The recycling system is introduced after the separation process, utilizing the residual ammonia vapor. This vapor is directed to a TEE, which serves to extract 1% of the stream as a purge. The remaining portion is routed back into the recycle stream. Subsequently, the recycled stream is passed through a compressor to elevate its pressure, ensuring it is equalized with the pressure required at the mixer inlet.

3. Result and Discussion

One of the most impactful strategies to improve energy efficiency in the Haber–Bosch ammonia synthesis process is the reduction of compressor workload, which directly influences energy demand for both compression and subsequent cooling [13]. Compressors typically require significant electrical energy to pressurize synthesis gas (a mixture of hydrogen and nitrogen), and as this pressure increases, so does the downstream requirement for intercoolers and heat exchangers to remove the associated heat of compression. In this study, a process simulation using Aspen HYSYS was conducted, where the synthesis gas pressure was gradually reduced to evaluate how it affects the overall energy consumption and reactor performance [14]. The central goal was to determine whether a lower operating pressure could maintain product conversion while reducing auxiliary energy demands.

The energy stream data summarized in Table 1 clearly demonstrates that this strategy leads to a substantial reduction in energy usage. Net energy consumption dropped from 6.53×10^7 kcal/h to 1.47×10^7 kcal/h after modification, indicating a 77.5% decrease in total energy requirement. This dramatic change can be traced to several key adjustments in the process. Notably, the cooling load on compressor K-100 (stream QC_{100}) fell significantly from 3.46E+7 kcal/h to 2.64E+7 kcal/h. Additionally, the secondary compressor (K-101) cooling duty (QC_{101}) dropped to a negligible 2.91E+5 kcal/h. These reductions highlight how decreasing compression pressure directly reduces heat generation, which in turn lowers the energy needed by the cooling systems, especially in the intercoolers and condenser units. Moreover, heat input into the system, reflected in QR_{100} and QE_{100} values, also shifted due to better thermal integration. QR_{100} increased in absolute value (i.e., more heat was released), while QE_{100}, representing energy entering the system, rose modestly, which suggests improved reactor efficiency under new conditions.

Supporting this analysis, the Aspen HYSYS Process Flow Diagram (PFD) shown in Figure 2 illustrates the detailed unit operations and flow directions within the system. Key units such as K-100 (main compressor), MIX-100 (mixer), E-100 (heat exchanger), CRV-100 (reactor), and V-100 (separator) are central to the energy flow and can be traced back to the data in Table 1. With reduced compression, less energy is required in the QC_{100} and QC_{101} streams, and the cooling load in QE_{101} also drops significantly. Importantly, the reactor maintained its vapor-phase operation, confirmed by a vapour fraction of 1, indicating that no condensation or phase instability occurred even at reduced pressures. This condition is essential because any condensation could disrupt

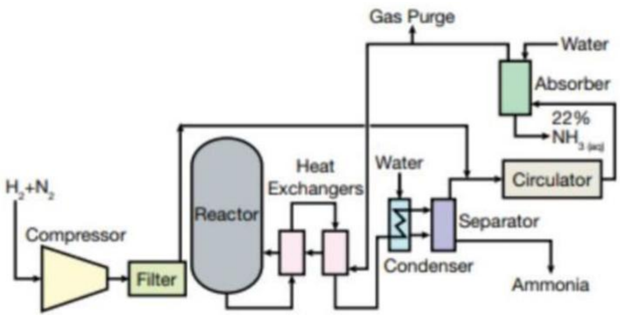

Figure 1. Basic process flow diagram (unmodified process).

Table 1. Comparison of energy streams before and after system modification in aspen hysys simulation.

Energy Streams	Unit	QC_{100}	QC_{101}	QR_{100}	QE_{100}	QE_{101}	Net Energy
Before Modification		3.46E+7		-1.80E+7	2.49E+7	2.39E+7	6.53E+7
Ater Modification	kcal/h	2.64E+7	2.91E+5	-4.59E+7	3.35E+7	3.08E+5	1.47E+7

the gas-phase kinetics of ammonia synthesis or cause operational difficulties in compressors and piping systems [15].

The process modification is also reflected in the simplified flowsheet diagram (Figure 3). This layout presents the process conceptually, clearly identifying energy exchange points such as $Q_{Kompresor}$, $Q_{cooler-1}$, $Q_{Reactor}$, and $Q_{Separator}$. These correspond with the heat duties reported in the simulation data. The flowsheet serves as a visual tool for understanding how the recycle compressor loop interacts with the reactor feed, and how thermal energy is managed across the system. The integration of recycle compression and improved temperature control through heat exchangers contributes to the overall energy efficiency of the redesigned process.

Beyond the numerical reduction in energy values, this strategy also brings important mechanical and economic benefits. Lowering the load on compressors reduces mechanical stress, extending the lifespan of these high-cost units. It also means that less electricity is needed to power the compressors, resulting in lower operating costs. The reduced thermal load on cooling systems means smaller or less intensive heat exchangers can be used, which may further reduce capital and maintenance costs. From a reliability perspective, the system becomes more robust due to lower pressure and temperature variations, reducing risks such as fatigue failure or fouling in heat exchangers.

In conclusion, the combined analysis of simulation data, process configuration (PFD), and conceptual flowsheet supports the effectiveness of pressure reduction as an energy-saving measure in ammonia production. The approach not only preserves reactor conversion and process stability but also delivers substantial savings in both cooling and compression energy. The successful integration of this strategy within Aspen HYSYS and the alignment with thermal and mechanical systems underscore its feasibility for real-world application. These results provide a solid foundation for further optimization involving pressure staging, heat recovery, and advanced control strategies to improve the sustainability of ammonia production processes.

A modification was made by reducing the operating pressure of compressor K-101 from 275 bar to 180 bar. This change aimed to improve the system's energy efficiency without compromising the product's output flow. Simulation results show that the net energy requirement decreased significantly from 4.14×10^{7} kcal/h to 1.47×10^{7} kcal/h, achieving an energy saving of approximately 64.5%. Despite the reduction in pressure, the molar flow rate of the product remained constant at 4857 kgmole/h, indicating a substantial increase in energy efficiency without

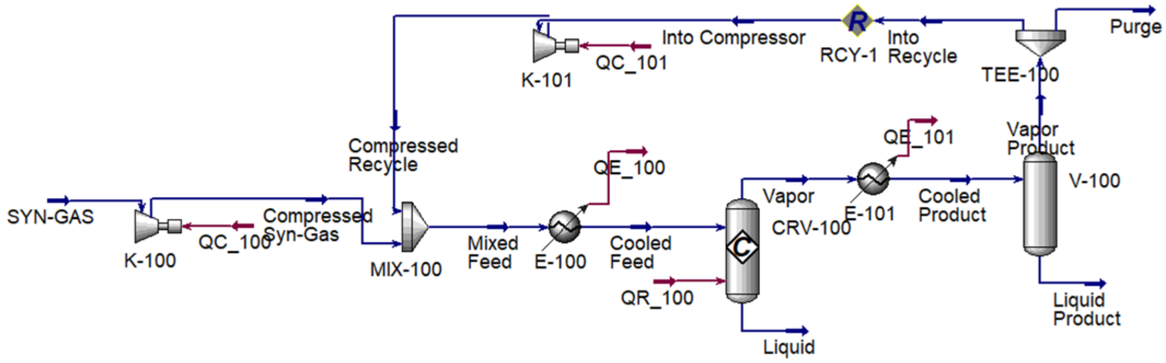

Figure 2. Aspen HYSYS process flow diagram after system modification.

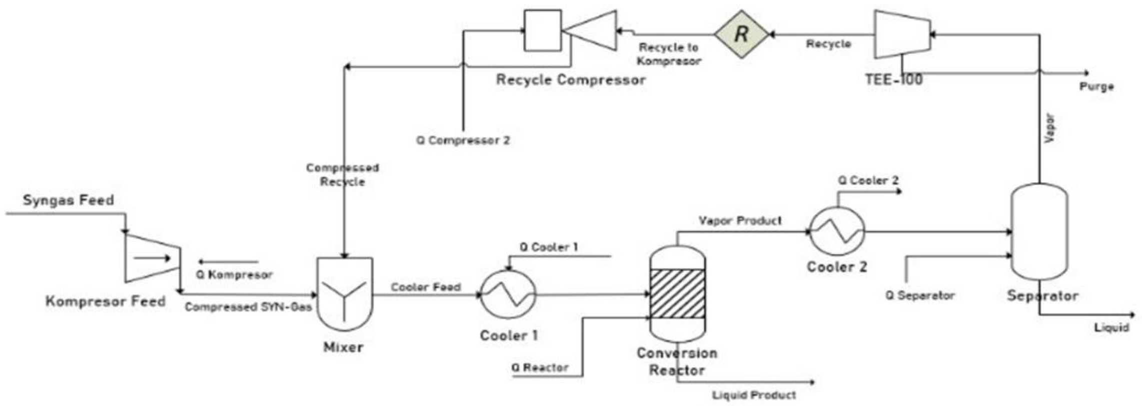

Figure 3. Conceptual Process Flow Diagram (PFD) of ammonia production.

sacrificing productivity. Therefore, the optimal operating condition is achieved at a pressure of 180 bar for compressor K-101, resulting in minimum net energy consumption while maintaining stable product output. The targeted improvement in energy efficiency was successfully achieved quantitatively through this pressure optimization.

4. Conclusion

System modifications in the ammonia production process led to a significant quantitative improvement in energy efficiency. Specifically, the net energy consumption dropped from 6.53×10^7 kcal/h to 1.47×10^7 kcal/h, representing a 77.5% reduction in total energy requirement. The cooling load on the main compressor (QC_{100}) decreased by 23.7%, from 3.46E+7 kcal/h to 2.64E+7 kcal/h, while the secondary compressor (QC_{101}) cooling duty was reduced by over 99%, dropped to a negligible 2.91E+5 kcal/h. These quantitative changes demonstrate that optimizing compression pressures and improving thermal integration can dramatically decrease the energy required for ammonia synthesis, thereby substantially enhancing overall production efficiency.

In conclusion, reducing the operating pressure in the ammonia production process proves to be an effective strategy for enhancing overall energy efficiency. This adjustment lowers the compressor workload, which in turn reduces system temperatures and eases the demand on the cooling system. Importantly, the process maintains a gas-phase reaction environment and high conversion efficiency, indicating that energy savings are achieved without compromising reaction performance. The results confirm that pressure optimization lies within the thermodynamic and kinetic boundaries necessary for effective ammonia synthesis.

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