

Simulation and Optimization of Ammonia Converter on Increasing the Mole Percent of Ammonia Products in the Ammonia Plant Through Modification Process

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Received: 12th December 2025; Revised: 15th December 2025; Accepted: 17th December 2025
Available online: 28th December 2025; Published regularly: December 2025



Abstract

Ammonia production efficiency is strongly influenced by temperature management within the multi-bed converter, where deviations from optimal conditions often reduce the final ammonia mole fraction compared to design expectations. To address this challenge, the ammonia synthesis loop was modified by adding a cooler and a heat exchanger between Bed-2A and Bed-2B to achieve more controlled inter-stage temperatures and improve equilibrium conversion. A complete process model was constructed in process simulation software using actual operating data, allowing evaluation of the original thermal profile and ammonia formation across each catalytic bed, followed by simulation of the modified configuration to quantify performance improvements. The optimized arrangement successfully increased the final ammonia mole fraction from 15.97% to 17.74%, approaching the design target of 19.02%, while maintaining temperatures closer to the ideal range for exothermic synthesis reactions. These results highlight that carefully targeted thermal adjustments and strategic heat integration can enhance reaction efficiency, reduce temperature-induced conversion losses, and provide a practical, implementable pathway for improving ammonia yield in existing industrial plants.

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Keywords: Ammonia Synthesis; Ammonia Converter; Heat Integration; Process Optimization

How to Cite: Hafidza, R. N., Soesilo, E. T. R., Bilbina, A. I., Ramadhani, A. M., Aqila, R. Y. (2025). Simulation and Optimization of Ammonia Converter on Increasing the Mole Percent of Ammonia Products in the Ammonia Plant Through Modification Process. *Journal of Chemical Engineering Research Progress*, 2 (2), 330-338 (doi: 10.9767/jcerp.20592)

Permalink/DOI: <https://doi.org/10.9767/jcerp.20592>

1. Introduction

Ammonia is a critical chemical compound that plays a key role in various industrial sectors, particularly as a primary raw material in nitrogen fertilizer production [1]. Ammonia production efficiency is highly dependent on ammonia conversion performance, which affects the ammonia content in the final product. In the ammonia production process, increasing the mole percentage of ammonia in the product can significantly improve plant productivity and energy efficiency [2]. However, achieving this requires appropriate process modifications and

improved reactor operating conditions. Ammonia has emerged as one of the most promising energy carriers for large-scale green hydrogen storage due to its high volumetric density, established global infrastructure, and compatibility with renewable energy pathways. Despite this potential, ammonia synthesis remains limited by the efficiency of its separation step, where conventional low temperature condensation restricts production rates and imposes substantial energy demands [3]. These limitations constrain their applicability in continuous, high-efficiency synthesis loops.

Ammonia is one of the most essential large-volume chemicals worldwide, with global annual production exceeding 180 million tons and growing steadily due to its critical role in fertilizer

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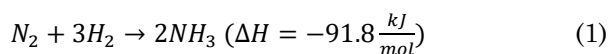
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manufacturing, energy storage, and emerging low-carbon fuel applications [4]. As a result, the performance of the ammonia converter, along with its associated heat-exchange network, strongly governs overall plant efficiency, specific energy consumption, and ammonia yield.

To maintain an optimal equilibrium profile, industrial converters commonly employ multi-bed catalytic configurations with inter-stage cooling. Effective temperature control is essential because excess heat causes the reaction equilibrium to shift backward, reducing ammonia formation [5]. Other researchers have utilized process simulators such as Aspen Plus or Aspen HYSYS to model reactor equilibrium, evaluate kinetic limitations, and analyze heat-integration opportunities. While these efforts have contributed to improved understanding of the synthesis loop, most previous works focus on isolated reactor optimization or steady-state equilibrium prediction without linking the complete thermal-hydraulic interactions represented in a process flow diagram (PFD). Furthermore, only a limited number of studies integrate actual plant operating data with a simulated PFD that explicitly incorporates cooler placement, inter-bed heat recovery, and exchanger duty analysis.

A few researchers have addressed converter improvement through enhanced heat-exchange configuration, yet comprehensive studies that reconstruct the ammonia synthesis loop using a detailed Aspen HYSYS generated PFD remain scarce. There is limited investigation on how modifications such as additional coolers or inter-stage heat exchangers influence inter-bed temperature control and ultimately affect ammonia outlet mole fraction under real plant operating conditions [6]. This gap is notable because even small deviations in temperature on the order of 5–10 °C may shift equilibrium conversion significantly, and inadequate thermal management can lower ammonia yield by more than 1–2 mol%, impacting daily production capacity.

The ammonia synthesis process takes place in an ammonia converter, a reactor where synthesis gas consisting of nitrogen (N₂) and hydrogen (H₂) is reacted to form ammonia (NH₃) through an equilibrium reaction that is highly exothermic [7]. The main reaction involved can be expressed as follows:



This process is based on the Haber-Bosch method, which operates under high temperature and pressure conditions, typically ranging from 400–500 °C and pressures of at least 100 bar. The

feed gas entering the reactor generally has a hydrogen-to-nitrogen ratio of approximately 3:1 [8]. In practice, this ratio may be slightly adjusted to achieve optimal operating conditions. Such adjustments can significantly influence the ammonia conversion rate, with the ammonia concentration in the reactor outlet gas typically ranging between 15–20 mol%. Unreacted gases are recycled back to the reactor to maximize overall production efficiency.

The converter used in this process is a horizontal intercooled type, where the feed gas passes through an interchanger prior to entering the reactor to increase its initial temperature [9]. This step helps maintain the temperature between catalyst beds, ensuring optimal conversion and achieving the desired outlet temperature. Inside the converter, an internal basket contains promoted iron catalyst arranged in multiple separate beds. These catalyst beds are divided into three sections: Bed-1, Bed-2A, dan Bed-2 to control the temperature rise caused by the exothermic reaction equilibrium toward the reactants, causing part of the produced ammonia to decompose back into N₂ and H₂. Therefore, temperature regulation through catalyst bed design and the use of quench gas streams is critical for maintaining conversion efficiency [10].

This research develops a rigorous simulation of the ammonia converter system using Aspen HYSYS, incorporating actual design and operating data to reconstruct the full process flow and evaluate the thermal behavior of each catalyst bed. The study systematically examines the effect of introducing additional cooling and heat-exchange units on inter-stage temperature control and equilibrium conversion. The objectives of this research are to construct a detailed Aspen HYSYS-based PFD of the ammonia synthesis loop, simulate the performance of each catalytic bed, and determine the extent to which heat-exchange modifications improve the final ammonia outlet mole fraction.

2. Methods

2.1 Process Simulation Software

In this study, Microsoft Visio was utilized to develop the Process Flow Diagram (PFD) representing the ammonia production process. The scope of process analysis requires handling numerous graphical representations of industrial operations. This task can be performed more effectively by utilizing an intuitive and efficient graphical modeling tool, particularly for designing accurate and detailed Process Flow Diagrams (PFD) that illustrate the sequence of equipment and material flows within the plant [11]. Furthermore, during the process simulation

stage, Aspen HYSYS is employed to model an industrial ammonia plant. The significance of real-time optimization for ammonia production is highlighted, along with the identification of decision variables, operational constraints, and their respective limits. While emerging technologies such as electrochemical and photocatalytic methods present promising alternatives, the Haber–Bosch process remains the core technology for ammonia synthesis, as outlined in the roadmap for the ammonia production [12].

2.2 Basic Process Flow Diagram

Figure 1 illustrates the basic flow diagram that serves as the conceptual foundation for the ammonia production process examined in this study. However, achieving maximum ammonia yield is hindered by losses occurring in the exhaust stream. To model the production process, the Peng–Robinson (PR) property package was applied [13]. This thermodynamic model was chosen due to its suitability for hydrocarbon-based systems and its ability to provide accurate predictions of phase equilibria, including gas–liquid, gas–liquid–liquid, and multicomponent mixtures. Consequently, the Peng–Robinson equation is regarded as highly appropriate for simulating the ammonia synthesis process [14].

2.3 Unmodified Method to Improve the Process

The process of the synthesis ammonia is using the multi-bed configuration. The feed gas, consisting of hydrogen, nitrogen, methane, argon, and residual ammonia, first passes through an interchanger, which functions as a heat exchanger to increase the feed temperature by utilizing heat recovered from the outlet stream of the first reactor bed. This energy integration step ensures that the feed enters Bed-1 at an optimal temperature for the exothermic Haber–Bosch reaction [15]. Bed-1, Bed-2A, and Bed-2B are fixed-bed catalytic reactors operating under high pressure and temperature conditions, where iron-based catalysts facilitate the conversion of nitrogen and hydrogen into ammonia. After leaving Bed-1, the partially converted gas flows to Bed-2A for further reaction. Due to the temperature drop caused by the exothermic nature of the reaction, the outlet stream from Bed-2A is reheated using a heater before entering Bed-2B, which completes the synthesis process. This multi-stage reactor arrangement, combined with intermediate heat recovery and reheating, is designed to maximize ammonia yield while maintaining thermal efficiency and catalyst performance.

2.4 Modification Method to Improve the Process

After passing through Bed-2A, the gas stream is not immediately reheated by a heater as in the first configuration; instead, it is first cooled using a cooler and then directed through a heat exchanger before entering Bed-2B. This approach enables more precise temperature control, ensuring that thermal conditions remain within the catalyst specifications and preventing degradation caused by excessive heat. Bed-2B continues to operate as a fixed-bed reactor to complete the ammonia synthesis reaction. The inclusion of a cooler and heat exchanger in this configuration reflects a greater emphasis on thermal optimization and energy efficiency compared to the previous system. It is known that the higher the inlet temperature, the lower the percentage of NH_3 obtained. An increase in system temperature shifts the equilibrium toward the left, which is the endothermic direction. This occurs because the ammonia synthesis reaction is exothermic; therefore, raising the temperature reduces the equilibrium concentration of ammonia and promotes the decomposition of NH_3 back into its reactants, H_2 and N_2 . Conversely, lowering the temperature shifts the equilibrium to the right, resulting in a higher ammonia yield [16]. Consequently, to achieve a high conversion rate, the reactor requires an integrated cooling system.

3. Results and Discussion

3.1 Process Flow Diagram of Ammonia Production Before Optimization

The process in the ammonia converter begins with the feed gas, which consists of hydrogen, nitrogen, argon, methane, and ammonia, being directed to the interchanger as depicted in Figure 1 and Figure 2. The ammonia converter feed exchanger (interchanger) serves to increase the temperature of the feed gas entering the ammonia converter by utilizing heat from the outlet gas of the converter itself. The interchanger is positioned at the beginning, before Bed-1, where the feed gas temperature is raised through heat exchange with the outlet gas from Bed-1. As a result, the outlet gas temperature from Bed-1 decreases before entering Bed-2A as feed and reacting to form ammonia. Subsequently, the outlet gas from Bed-2A is directed to a heater to increase its temperature in order to maximize the ammonia formation process in Bed-2B.

Based on Table 1, the mol percentage of NH_3 obtained from the design data is 17.02%, while the average mol percentage of NH_3 obtained from the actual data is 15.973%. The highest mol percentage of NH_3 in the actual data during the observation period occurred in the 9th data, which

was only 0.2 different from the design data (98.82% close to the design). Meanwhile, the lowest molar percentage of ammonia was obtained in the 10th data, which had a difference of 1.74 from the design data (89.77% close to the design). The ammonia percentage obtained in the actual data was lower and did not match the design data. This could be caused by several factors, one of which was the inlet temperature of the converter or the inlet temperature of each bed.

The highest NH₃ percentage in data point 9, at 16.82% mol, has an inlet temperature value of 259.1 °C. The NH₃ percentage in this data point is lower than in the design data. This indicates that the inlet temperature value affects the percentage of NH₃ mol produced. The higher the inlet temperature, the lower the mol% of NH₃ obtained. When the system temperature rises, the equilibrium shifts to the left (endothermic) [17]. As in data point 10, which has the highest inlet

temperature of 260.7 °C but produces the lowest NH₃ percentage of 15.28%.

Based on the comparison between the design and actual operating data, the consistently lower NH₃ mol percentages in the plant indicate that the existing operating conditions particularly the converter inlet temperature—are not optimal for achieving the intended ammonia yield. Since higher inlet temperatures shift the reaction equilibrium toward the reactants and reduce ammonia formation, as observed in data points 9 and 10, adjusting these conditions becomes necessary to enhance performance. Therefore, modifying the process and altering key operating parameters such as converter inlet temperature are justified steps to move the system closer to the design equilibrium conditions, minimize deviations, and ultimately increase the ammonia mol percentage produced.

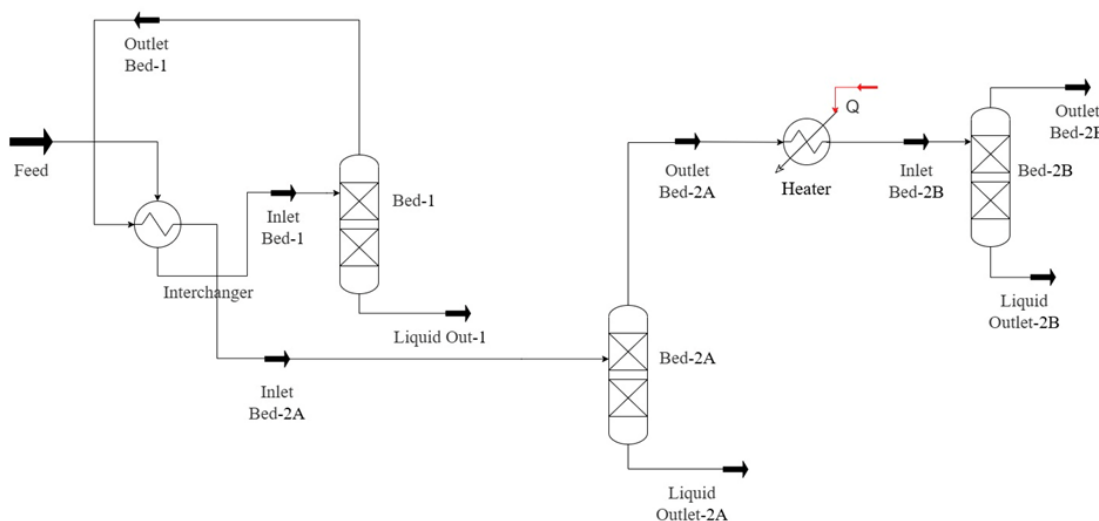


Figure 1. Basic process flow diagram (PFD) scheme of the ammonia converter.

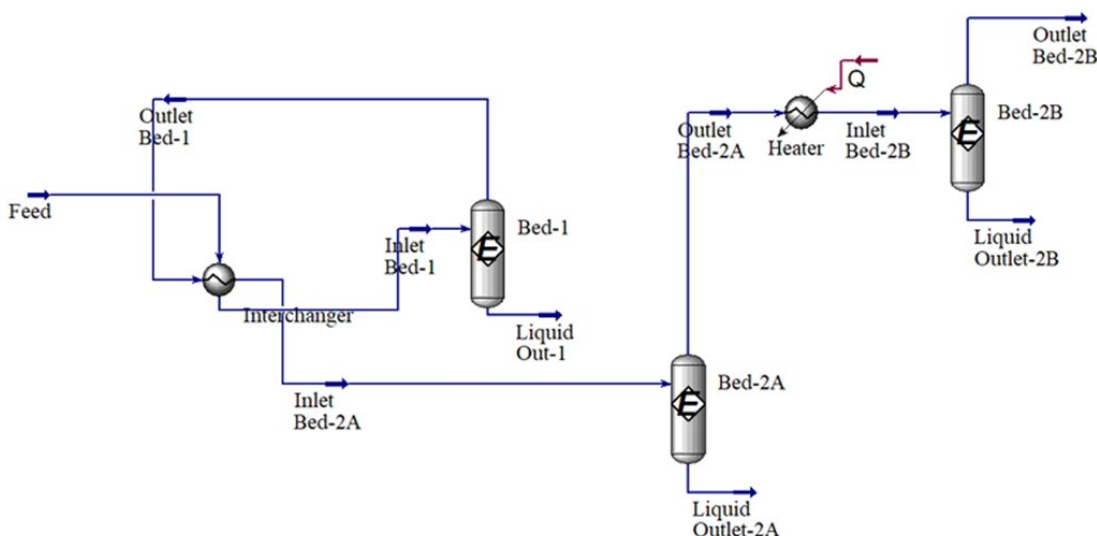


Figure 2. Process simulation of the ammonia converter using simulated Aspen HYSYS.

3.2 Process Flow Diagram of Ammonia Production after Optimization

The optimization process of the ammonia converter in Figures 3 and 4 involves the same stages as the process in Figure 2, where the feed gas is fed into the interchanger to increase its temperature and then reacts in bed-1. The gas outlet from bed-1 decreases before entering bed-2A as feed and reacting to form ammonia. However, the difference lies in the addition of heat exchange instruments, namely a cooler and a heat exchanger, between bed-2A and bed-2B. The cooler is located after bed-2A so that the temperature of the gas outlet from bed-2A decreases, and then the gas is fed into the heat exchanger for heat exchange with the outlet from bed-2B. This aims to maximize the ammonia formation process in bed-2B.

Based on Table 2, the mol percentage of NH₃ obtained from the design data is 19.02%, while the average NH₃ percentage obtained from the actual

data is 17.738%. It is explained that an optimal converter temperature profile can increase fractional conversion by 42.38% and ammonia conversion by 56.48%. This indicates that the final mol percentage of ammonia in both the design and actual data has increased due to the addition of a cooler and heat exchanger between beds 2A and 2B. The highest NH₃ percentage in the actual data during the observation period occurred in the 7th data, which was only 0.33 different from the design data (98.265%, close to the design). Meanwhile, the lowest molar percentage of ammonia was obtained in the 1st data, which was 2.65 different from the design data (86.0673%, close to the design).

When viewed from the process prior to optimization, the actual data for the 9th sample showed a decrease in product percentage. This was due to the influence of temperature. The temperature required for the reaction to occur exceeded the optimum limit, causing the reaction to shift to the left, i.e., towards the reactants.

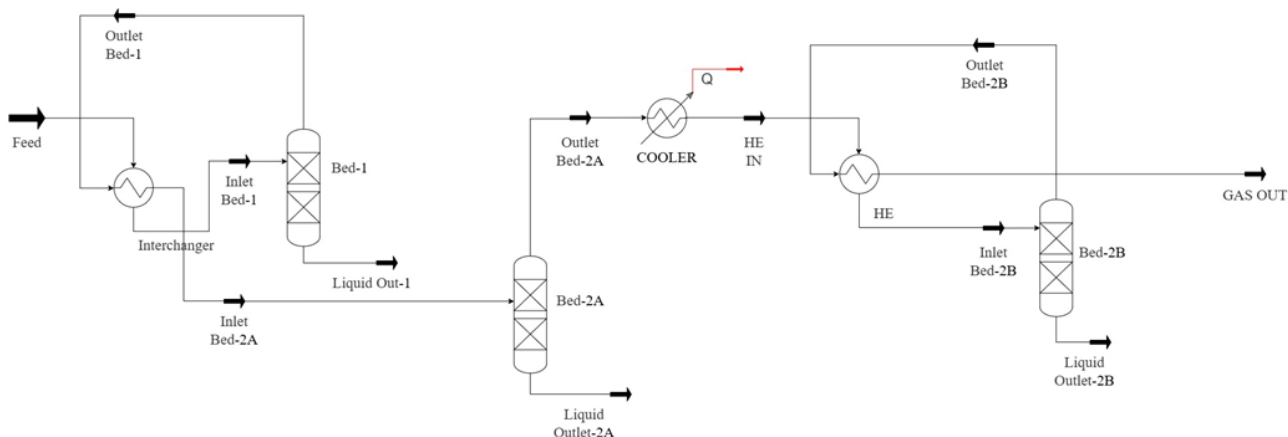


Figure 3. Basic process flow diagram (PFD) scheme of the ammonia converter.

Table 1. Percent mol NH₃ comparison in ammonia converter of each bed before optimization

Data	T _{in} Bed-1 (°C)	NH ₃ Out Bed-1 (%mol)	T _{in} Bed-2A (°C)	NH ₃ Out Bed-2A (%mol)	T _{in} Bed-2B (°C)	NH ₃ Out Bed-2B (%mol)
Actual Design	352.0	11.78	378.5	17.35	460.0	17.02
1	371.9	10.87	380.8	16.32	462.7	15.90
2	372.3	10.65	388.0	15.74	465.6	15.34
3	367.5	11.36	388.0	16.73	465.4	16.07
4	333.8	12.57	408.0	16.12	455.0	16.06
5	372.3	10.74	381.9	16.08	451.0	16.26
6	369.3	10.81	380.7	16.05	451.3	16.05
7	372.3	10.85	380.7	16.01	448.2	16.26
8	373.5	10.77	391.0	15.77	459.0	15.69
9	374.5	10.81	390.6	15.76	434.7	16.82
10	376.5	10.77	391.5	15.73	466.3	15.28
Average						15.973

Ammonia conversion increased with rising temperature, but at a certain temperature, the shift in chemical equilibrium began to dominate. This means that there is an optimum point where the maximum amount of ammonia is obtained [18]. Increasing the inlet temperature beyond the optimum point results in a decrease in conversion [17]. This shows that in exothermic reactions, when the temperature exceeds the threshold, productivity decreases, and the product decomposes into reactants until equilibrium is reached [19].

In addition, the temperature during the ammonia formation process can affect the reaction rate. Higher temperatures cause particles to move more frequently, thereby increasing the frequency and rate of collisions [20]. However, if the temperature used is very low, the reaction rate decreases. The formation rate initially increases with increasing temperature but then reaches a maximum when the system approaches thermodynamic equilibrium [21]. Therefore, the temperature

must be optimized to obtain a better reaction rate. Meanwhile, other factors such as pressure in this optimization process have no effect because the pressure of the gas is constant.

3.3 Effect of Adding a Cooler to an Ammonia Converter

The effect of adding a cooler to an ammonia converter is that it can increase ammonia conversion by lowering the reaction temperature, thereby making the reaction faster and more efficient. This leads to an increase in the conversion of nitrogen and hydrogen gas into ammonia. The ammonia production reaction is an exothermic reaction, i.e., a reaction that releases heat. High reaction temperatures can cause the reaction to proceed more quickly, but they can also cause the reaction to be incomplete [20]. This is because at high temperatures, some of the nitrogen and hydrogen can react to form other undesirable compounds, such as nitrogen oxide (NO) and carbon monoxide (CO) [21].

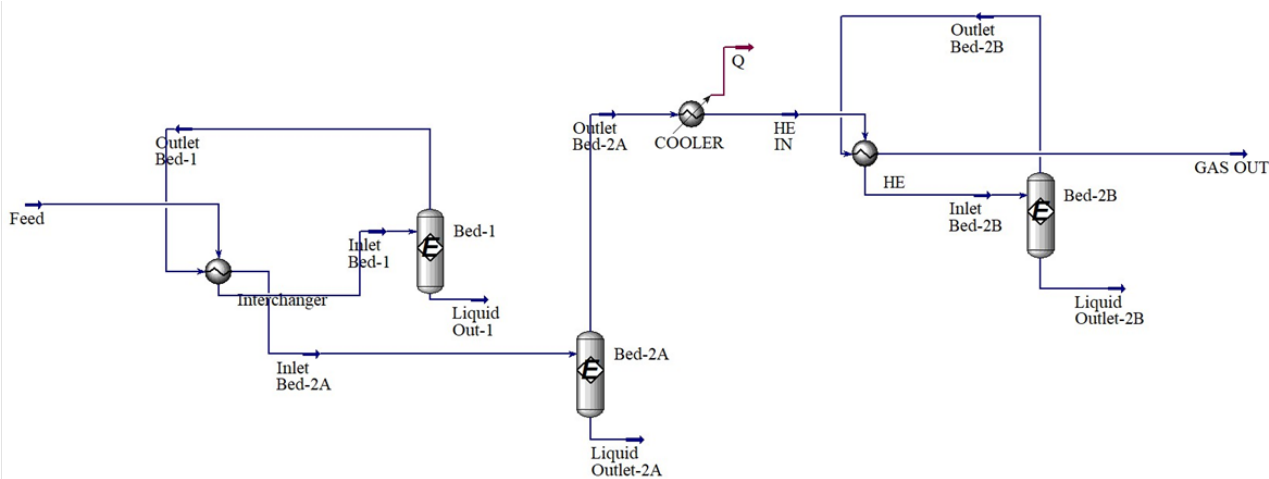


Figure 4. Process simulation of the ammonia converter after optimization using Aspen HYSYS

Table 2. Percent mol NH₃ comparison in ammonia converter of each bed after optimization.

Data	Tin Bed-1 (°C)	NH ₃ Out Bed-1 (%mol)	Tin Bed-2A (°C)	NH ₃ Out Bed-2A (%mol)	Tin Bed-2B (°C)	NH ₃ Out Bed-2B (%mol)
Actual Design	352.0	11.78	378.5	17.35	420.0	19.02
1	371.9	10.87	380.8	16.32	453.0	16.37
2	372.3	10.65	388.0	15.74	420.0	17.55
3	367.5	11.36	388.0	16.73	420.0	18.33
4	333.8	12.57	408.0	16.12	420.0	17.81
5	372.3	10.74	381.9	16.08	410.0	18.29
6	369.3	10.81	380.7	16.05	430.0	17.09
7	372.3	10.85	380.7	16.01	400.0	18.69
8	373.5	10.77	391.0	15.77	410.0	18.12
9	374.5	10.81	390.6	15.76	444.0	16.56
10	376.5	10.77	391.5	15.73	400.0	18.57
Average						17.738

The decrease in the outlet temperature of the converter bed with the addition of a cooler can absorb the heat of the reaction, thereby lowering the outlet temperature of the converter bed. This can reduce the risk of damage to the converter equipment due to overheating. Overheating occurs because at high temperatures, metals used to make converters can expand and change shape.

The effect of increasing energy efficiency by adding a cooler can save the energy needed to cool the gas flow [1]. This can increase the energy efficiency of the ammonia production process. The process of cooling the gas flow in the ammonia converter requires a significant amount of energy. Overall, adding a cooler to the ammonia converter can increase ammonia conversion, lower the converter bed outlet temperature, and increase energy efficiency.

3.4 Effect of Adding a Heat exchanger to an Ammonia Converter

The outlet gas from bed-2A, after passing through the cooler, is directed to a heat exchanger where it exchanges heat with the outlet gas from bed-2B. The primary function of this heat exchanger is to raise the temperature of the gas entering bed-2B by utilizing the thermal energy of the bed-2B outlet stream. As a result, the outlet gas temperature from the ammonia converter remains moderate before entering the subsequent cooling stage. Based on Table 2, optimization led to a significant reduction in the outlet gas temperature compared to pre-optimization conditions. This demonstrates that the use of a heat exchanger not only lowers the converter outlet temperature but also increases the mole fraction of ammonia produced [22]. Furthermore, the heat exchanger ensures that the inlet gas temperature to each bed remains stable [23].

From a thermodynamic perspective, increasing temperature shifts the equilibrium toward the endothermic direction, thereby lowering the temperature [24]. At higher temperatures, the equilibrium moves to the left, reducing ammonia yield. Although operating at lower temperatures may appear advantageous for maximizing ammonia production, it simultaneously slows the reaction rate. The heat exchanger therefore enhances the performance of the ammonia converter by elevating the temperature of the gas entering bed-2B. The process simulation of the ammonia converter incorporating a cooler between the reactor beds is illustrated in Figure 5, which demonstrates the role of direct cooling in reducing the outlet temperature of the gas stream before it enters the subsequent bed. In contrast, Figure 6 presents the process simulation of the ammonia converter with the addition of a heat exchanger, highlighting an alternative strategy that utilizes internal heat recovery to regulate the inlet temperature of bed-2B.

The heat exchanger employed is of the shell-and-tube type, in which one fluid flows through the tubes while the other passes through the shell surrounding them. In this optimization process, the input gas to the heat exchanger is directed to the shell side, while the bed-2B outlet gas flows through the tube side. The simulation model applied is a simple end-point type, assuming no phase change, a constant overall heat transfer coefficient, and negligible heat loss.

4. Conclusion

This study successfully addressed its objective of enhancing ammonia converter performance by introducing a cooler and heat exchanger between Bed-2A and Bed-2B, resulting

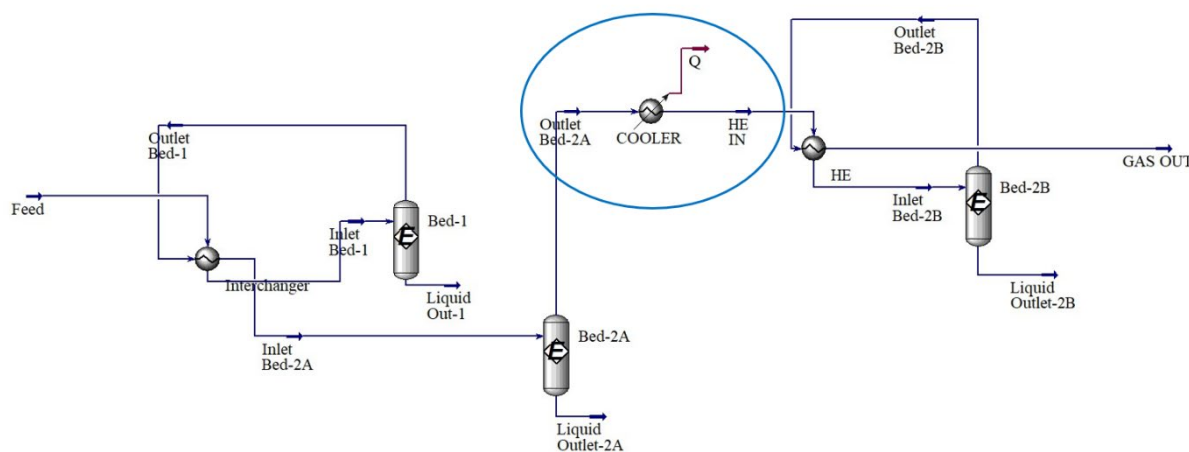


Figure 5. Process simulation of the ammonia converter with the addition of a cooler using Aspen HYSYS

in a measurable increase in ammonia mole fraction from 15.97% to 17.74%, approaching the design target of 19.02%. Based on the study, it is explained that an optimal converter temperature profile can increase fractional conversion by 42.38% and ammonia conversion by 56.48%. By integrating thermal management strategies into the synthesis loop, this work advances current knowledge beyond conventional multi-bed configurations, demonstrating that precise temperature control can significantly improve equilibrium conversion and energy efficiency. These findings provide a practical pathway for optimizing ammonia production in industrial plants and support its role as a sustainable energy carrier for green hydrogen storage. Future research should explore the combined effects of pressure adjustments, advanced catalyst formulations, and dynamic optimization under variable load conditions. Experimental validation of these modifications at pilot scale and integration with renewable energy systems are underway to further strengthen the applicability of this approach.

CRedit Author Statement

Author Contributions: R.N. Hafidza: Validation, Writing Draft Preparation, Project Administration, Visualization; E. Soesilo: Conceptualization, Methodology, Formal Analysis, Writing Draft Preparation, Validation, Investigation, Supervision; A. I. Bilbina: Conceptualization, Validation, Resources, Writing Draft Preparation, Project Administration; A. M. Ramadani: Software, Data Curation, Writing Draft Preparation; R.Y. Aqila: Software, Data Curation, Writing Draft Preparation. All authors have read and agreed to the published version of the manuscript.

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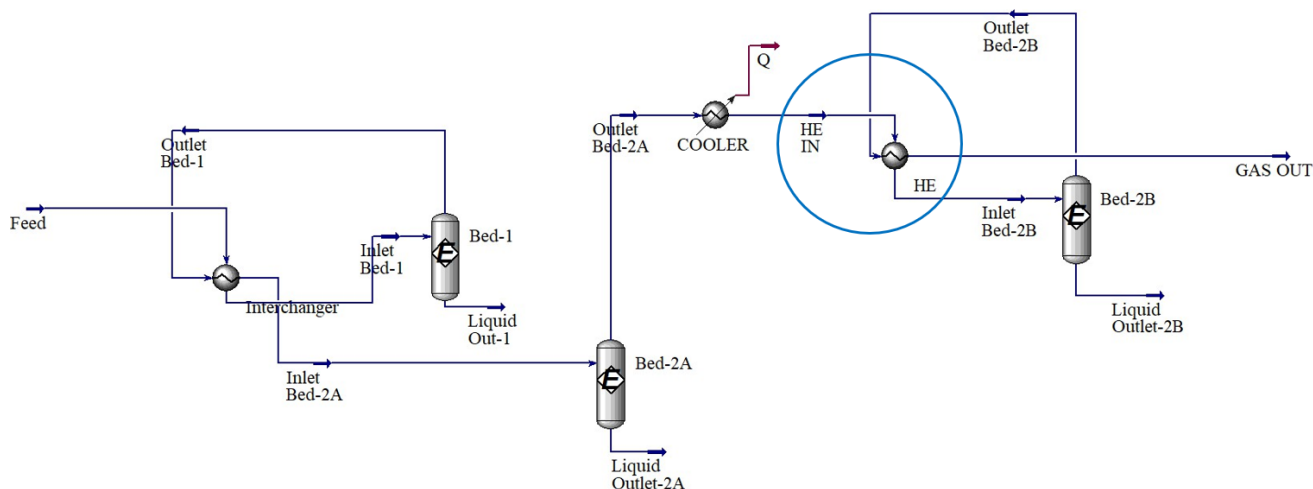


Figure 6. Process simulation of the ammonia converter with the addition of a heat exchanger using Aspen HYSYS

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