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Research Article

Performance Analysis of Ammonia Converter in Ammonia Unit Factory

Evaluasi Kinerja Ammonia Converter Pada Pabrik Unit Amonia

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Abstract

An ammonia converter is a catalyzed reactor that facilitates the synthesis of NH_3 (ammonia) from hydrogen (H_2) and nitrogen (N_2). Several studies have shown that the performance of this reactor significantly influences the operational efficiency and productivity of ammonia plants. Therefore, this study aims to evaluate the performance of an ammonia converter by assessing the effect of operating conditions on the reactant conversion and reaction products using design and actual data. The operating conditions examined included temperature, pressure, ratio of reactants, and inert mole utilized during the NH_3 synthesis process. The results showed that the highest NH_3 yield of 20.28% was achieved in actual data with 351.5^{o}C temperature, 154.32 kg/cm^2 pressure, 3.58 raw material ratio, and 3.57% inert mole (sixth dataset). The performance efficiency of an ammonia converter can be assessed using temperature, reactant ratio, and inert moles, while the pressure factor was insignificant due to dataset fluctuations. Based on the evaluation results, the converter experienced a decrease in performance due to a discrepancy in the existing operating conditions between the design and actual data.

Keywords: Ammonia converter; operating conditions; reactor; yield

Abstrak

Ammonia Converter adalah reaktor berkatalis yang berfungsi sebagai tempat proses pembentukan NH_3 *(amonia) dari hidrogen* (H_2) *dan nitrogen* (N_2)*. Reaktor ammonia converter sangat berpengaruh terhadap produktivitas dan efisiensi di pabrik amonia sehingga diperlukan analisis kinerja reaktor. Tujuan penelitian ini untuk mengevaluasi kinerja ammonia converter berdasarkan kondisi operasi terhadap hasil konversi reaktan dan produk reaksi yang dihasilkan dengan ditinjau dari data desain dan data aktualnya. Penelitian ini menganalisis kondisi operasi suhu, tekanan dan rasio reaktan serta inert yang dihasilkan dari proses sintesis* NH_3 *dengan membandingkan data aktual yang didapatkan dengan data desainnya. Hasil evaluasi menunjukkan kondisi operasi optimal yang dicapai oleh* NH_3 *converter dengan suhu 154,32*^{o}*C, tekanan 154,32 kg/cm*^{2}*, rasio reaktan 3,58 dan mol inert 3,57% dengan konversi* H_2 *32,82%, konversi* N_2 *35,11% dan yield* NH_3 *20,28%. Hasil evaluasi menujukkan efisiensi kinerja reaktor ammonia converter dapat ditinjau oleh suhu, rasio reaktan dan mol inert sedangkan faktor tekanan tidak dapat digunakan karena data aktualnya yang fluktuatif.*

Kata kunci : *Ammonia converter; kondisi operasi; reaktor; yield*

1. Introduction

Ammonia synthesis is a process that is often carried out in an ammonia converter unit. Within this unit, synthesis gases (N_2 and H_2) obtained from the purification unit are reacted to obtain ammonia based products [1]. Furthermore, it is indigenously structured with three horizontal bed converters, which are designed using pressure wall materials at a cold temperature. The cold feed gas is passed through the annulus between the catalyst basket and the converter wall to maintain a low wall vessel temperature [2,3]. The converter unit also consists of a removable basket containing 4 fixed beds and 2 interchangers, with approximately 77.1 m^3 of promoted iron catalyst [3]. The volume of the catalyst within the beds varies, and it increases from the first to the third bed. This strategic volume augmentation helps to curtail the temperature elevation caused by the exothermic reaction occurring within the first bed (where the fastest reaction occurs). Consequently, the design preserves the converter's temperature within the desired range [3,4]. The ammonia formation is an exothermic equilibrium reaction using the Haber-Bosch process method, which is illustrated below [1]:

$$N_{2(g)} + 3H_{2(g)} \rightleftarrows 2NH_{3(g)} \quad \text{.....................}\mathbf{(1)}$$

The performance of an ammonia converter is significantly influenced by several factors, including temperature, pressure, H_2/N_2 ratio, and inert mole. Several studies have shown that temperature plays a dual role, impacting both the synthesis reaction rate and ammonia equilibrium. NH_3 synthesis occurs through an exothermic reaction, leading to the limitation of the operating temperature by chemical equilibrium. However, higher levels concurrently enhance kinetic energy, leading to faster molecular collisions [5].

Pressure is a crucial factor that influences both the equilibrium of NH_3 and reaction rate, where higher levels often lead to increased yield. Changing the H_2/N_2 ratio can lead to an increase or decrease in yield in an ammonia converter. Based on the plant design, an optimal H_2/N_2 ratio typically ranges from 2.8-3.2 [2–4]. The primary operational variable used to control the hydrogen and nitrogen ratio is the composition of the introduced make-up or fresh feed gas.

Methane and argon are inert components commonly found within the syngas stream. These components are not harmful to the catalyst and do not undergo synthesis reactions. However, they have been reported to have a negative impact on reaction rates and equilibrium. A feasible approach that is often used to minimize inert concentration involves purging syngas in the loop [1,3,4]. Therefore, this study aims to analyze the performance of an ammonia converter in an NH_3 plant by comparing the yield obtained under actual and standard operating conditions. The parameters observed included temperature, pressure, reactant ratio, and the inert mole produced by the reactor.

2. Research Methods

The methodology used in this study included a literature review, observation, as well as data collection and processing. The dataset used for the ammonia converter analysis consisted of both design and actual data. The design dataset included the predetermined parameters established during the development of the unit [2,4]. Furthermore, these parameters consisted of inlet temperature, pressure, inert mole, and H_2/N_2 reactant ratio.

3. Results and Discussion

The actual data used for evaluating the performance of an ammonia converter were obtained from the operation conditions at the control room and laboratory of the PT PUSRI IIB unit in the form of log sheets. The conditions examined included the flow rate, %mol composition data for inlet and outlet, feed temperature, pressure, inter-bed temperature, inert mole, and H_2/N_2 reactant ratio. Furthermore, the analysis was performed with mass balance calculations using Microsoft Excel to determine the conversion of N_2 and H_2. It was also used to determine the yield of NH_3 products produced by comparing the design and actual data. The actual data from 6th December 2021 to 31th January 2022, were used, totaling 9 dataset points.

Table 1 shows the results of H_2 and N_2 reactant conversion as well as NH_3 yield based on the operating conditions of temperature, pressure, reactant ratio, and inert mole. The data were then plotted as a graph in Figure 1 to observe the midpoint of the dataset points based on the conditions influencing the reactant conversion and product yield. Polynomial regression was performed on the data in Table 1 to determine the optimal relationship between temperature, pressure, reactant ratio, and an inert mole in the conversion of H_2 and N_2 into NH_3.

In Figure 1, there was a convergence point of the four sets of operating conditions, which was indicated by the 6th dataset. This suggested that the optimal operating conditions affecting the NH_3 production process were achieved with the 6th data, namely 351.25 °C temperature, 154.32 kg/cm^2 pressure, 3.58 reactant ratio, and 3.57% inert mole.

Based on polynomial regression results, Figure 2 showed a similar intersection point to Figure 1, which was achieved at the 6th operating data point. This indicated the occurrence of synchronization between the factors affecting the NH_3 process, namely temperature, pressure, reactant ratio, and inert mole. The conversion results obtained were 32.82% conversion of H_2, 35.11% conversion of N_2, and 20.28% yield of NH_3.

Table 1. Ammonia Converter Operating Conditions: Design and Actual Data

Data	Inlet Temp. (°C)	Inlet Press. (kg/cm^2)	H_2/N_2 Ratio	Inert (%mol)	Energy Gibbs (kJ/kmol)	H_2 Conversion (%mol)	N_2 Conversion (%mol)	NH_3 Yield (%mol)
1	349,50	151,84	3,20	3,78	-165,9	30,00	33,11	19,56
2	349,31	152,57	3,31	3,68	-165,9	30,85	34,30	19,92
3	349,34	153,40	3,37	3,63	-165,9	28,41	36,66	20,10
4	347,73	153,61	3,57	3,61	-165,6	32,91	34,15	19,89
5	347,56	155,02	3,34	3,78	-165,6	29,04	36,11	20,11
6	351,25	154,32	3,58	3,57	-166,3	32,82	35,11	20,28
7	348,42	154,45	3,55	3,68	-165,7	30,57	35,71	20,05
8	347,75	154,80	3,43	3,57	-165,6	25,00	38,66	19,78
9	349,25	154,40	3,26	3,80	-165,9	31,13	33,61	20,03
Design	**380,00**	**157,90**	**3,00**	**3,50**	**-171,8**	**32,55**	**32,44**	**20,31**

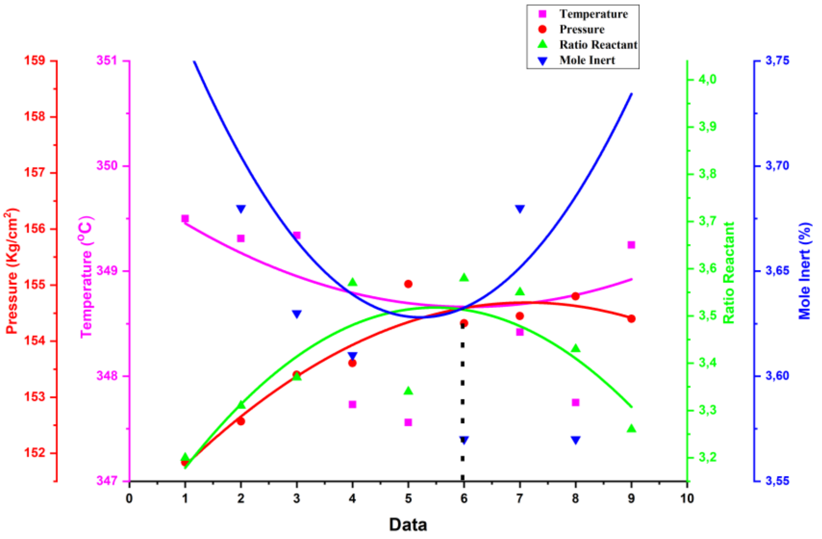

Figure 1. Comparison of temperature, pressure, reactant ratio, and inert mol toward operating data 1-9

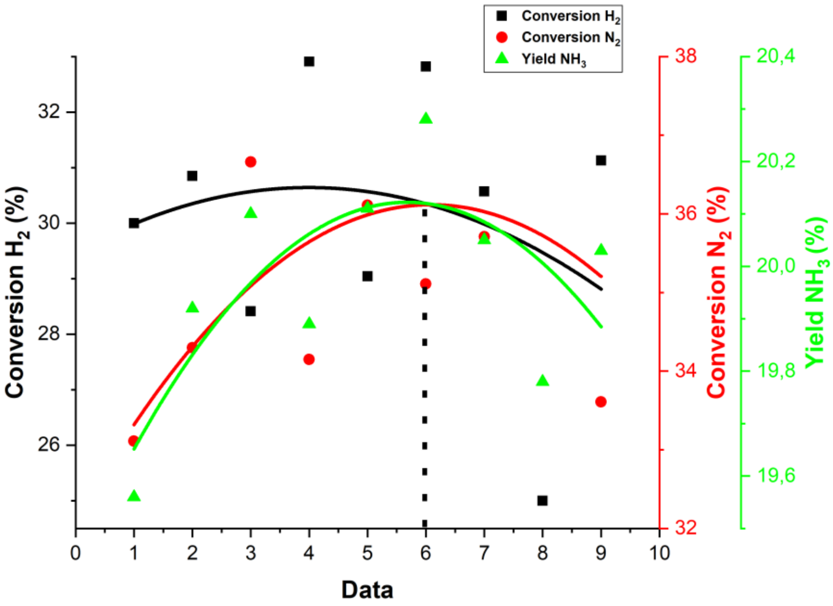

Figure 2. Comparison of H_2 conversion, N_2 conversion, and NH_3 yield toward operating data 1-9

The optimal temperature in this study was 351.25°C, leading to an NH_3 yield of 20.28% and an H_2 reactant conversion of 32.82%, which were the highest actual data. This study showed that the actual dataset results were similar to the design results, as shown in Table 1. Furthermore, high reaction temperatures could yield high reactant conversion and product yield [6]. Operations at high levels often accelerated the reaction process and increase the conversion of H_2, N_2, and mole NH_3 [7]. However, processes at high temperatures could shorten the catalyst lifespan by causing faster saturation and decreasing the NH_3 equilibrium degree in the reaction [8].

Inlet temperature affected the NH_3 yield through two factors, including chemical equilibrium and chemical kinetics. Based on chemical equilibrium, the effect of these factors was governed by Le Chatelier's principle. The principle stated that a system in equilibrium, when affected externally, shifted to form a new equilibrium to minimize the external effect [9]. This indicated that the operating temperature in exothermic reactions was limited by chemical equilibrium. When the levels exceeded the threshold, productivity decreased, and product decomposition into reactants occurred to reach a balance [10]. Therefore, the operating temperature in the NH_3 reaction must be maintained within the desired range.

The decrease and increase in NH_3 yield with temperature could be attributed to the energy involved in the reaction process, specifically Gibbs energy [11]. Gibbs energy is a measure of the potential work of a reversible reaction or the maximum work possible for a system at a constant temperature or pressure [11, 12]. Furthermore, it was often used to assess the spontaneity of a reaction. Equilibrium occurred when its value was zero, and there was no reaction if the value was greater than zero. This indicated that the smaller the generated Gibbs energy, the higher the negativity, leading to increased spontaneity [13].

Factors in chemical reaction kinetics were related to the rate of reaction. Higher temperatures often led to faster reactions, leading to an increase in product formation [14]. This was because higher temperatures led to more frequent particle movement, thereby increasing collision frequency and rate [15]. Therefore, increasing the levels within the equilibrium limit could enhance the NH_3 product yield. For the Haber-Bosch synthesis of NH_3, the chemical equilibrium limit occurred at a temperature of 495°C [13].

Decreases in yield were also affected by catalyst performance in each bed and interchanger performance. A lower inlet temperature for an ammonia converter increased the load on the interchanger to raise the level to the desired range. This was because an ammonia converter reaction was exothermic, indicating that increased the temperature enhanced raw material yield, but decreased the NH3 equilibrium degree in the reaction [16].

Optimal conditions were achieved at the 6th data point with a pressure of 154.32 kg/cm^2. This actual value was lower compared to the design data of 157.9 kg/cm^2. The results showed that pressure affected both NH_3 equilibrium and reaction rate [16,17].

The increased pressure was caused by several factors, such as the flow rate of fresh makeup gas, a decrease in converter temperature below the desired range, and changes in the gas composition of the H_2 and N_2 ratios. It could also be caused by an increase in NH_3 content in the recycle gas, an increment in inert content, and catalyst deactivation [18], leading to a reduction in product yield. This aligned with the actual data obtained from the first data point with the lowest pressure of 151.84 kg/cm^2, which yielded the smallest N_2 conversion at 33.11% and NH_3 mol composition at 19.56%. However, this could not be proven for H_2 conversion data due to its greater fluctuation compared to others.

The optimal reactant ratio of 3.58 was achieved at the 6th data point, which was higher compared to the design dataset of 3. Furthermore, the H_2/N_2 ratio referred to the ratio of H_2 and N_2 inlet for each reactant. In the 6th data point, with a value of 3.58, the H_2 conversion was closest to the design data. This corresponded to the highest NH_3 yield obtained from the actual data at 20.28%.

The relationship between the H_2/N_2 reactant ratio and NH_3 yield was related to concentration. According to Le Chatelier's principle, when the equilibrium system experienced an increase in concentration on one side, the equilibrium shifted to the opposite side [19]. Therefore, increasing the raw material H_2/N_2 ratio was expected to lead to an increase in NH_3 product yield [20].

During the synthesis process, 3 molecules of H_2 and 1 molecule of N_2 were needed to form 2 molecules of NH_3. When the H_2/N_2 ratio increased beyond the limit, an imbalance in the reactant ratio occurred [21]. Therefore, control of this parameter was necessary to achieve the desired product yield.

In an ammonia converter, the H_2/N_2 ratio was easier to maintain compared to controlling the temperature and pressure conditions. Furthermore, it could be maintained in the reforming unit, specifically in the secondary reformer, by adjusting the air supply to maintain a close-to-3:1 H_2/N_2 ratio.

H_2/N_2 ratio greater than 3 could be controlled by increasing the airflow into the secondary reformer to increase N_2 as the feed for an ammonia converter. H_2 and N_2 components were maintained since the reactants flowed into an ammonia converter or as fresh feed gas to be converted into NH_3.

Figures 1 and 2 showed the optimal conditions achieved at the 6th data point, with an actual inert mol of 3.57%, which was the closest to the design value of 3.5%. This inert mole gave the highest NH_3 yield and was closest to the design data at 20.28%. Furthermore, the results showed that an increase in the parameter reduced the total reactant conversion. Although the inert compounds present in an ammonia converter were not catalyst poisons, the percentage of inlet and outlet inert mol increased in actual conditions [21]. The increase in the parameter reduced the amount of raw materials entering an ammonia converter. Changes in the percentage value of inert mol in actual conditions were affected by the performance of the reforming section, which supplied reactants before entering the reactor. Methane carried into the converter was obtained from the reactants in the primary and secondary reformers that were not converted into H_2 raw materials.

4. Conclusion

In conclusion, the evaluation of the NH_3 reactor performance showed optimal operating conditions, namely 351.25°C temperature, 154.32 kg/cm^2 pressure, 3.58 reactant ratio, and 3.7% inert mol. These operating conditions gave the highest NH_3 yield at 20.28%, with 32.82% H_2 conversion and 35.11% N_2 conversion. However, the pressure factor was difficult to evaluate due to the fluctuating and unstable data obtained.

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