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Ammonia Decomposition: A Route to Decentralized Hydrogen Generation

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Hydrogen, a zero-carbon energy carrier, is essential for achieving a sustainable future. However, its widespread utilization is hindered by challenges related to storage and transportation. Ammonia, a hydrogen-rich compound, emerges as a promising alternative due to its high energy density, ease of liquefaction, and safe handling. This research investigates the potential of producing high-purity hydrogen through the decomposition of ammonia. Process simulation using Aspen Plus® software was employed to evaluate the thermodynamic feasibility and energy efficiency of the system. The simulation framework includes catalytic ammonia cracking and hydrogen compression up to 350 bar. Also, a comprehensive techno-economic analysis was conducted to assess the economic viability of the proposed process compared to traditional hydrogen production methods. The analysis incorporated factors such as capital expenditure (CAPEX), operating expenditure (OPEX), and the levelized cost of hydrogen (LCOH). The compression cost represents the most significant portion, 44 %, followed by the hydrogen purification unit, which accounts for 26 % of CAPEX. Economic analysis based on process simulation estimates the unit cost of hydrogen at 6.57 \$/kg H_2 for a Hydrogen Refueling Station (HRS) with a production rate of 400 kg H_2/d.

1. Introduction

The development and commercialization of clean, sustainable energy technologies aim to reduce the impacts of global warming. Renewable energy emerges as a key solution to counter the environmental harm caused by widespread fossil fuel consumption. However, power generation from renewable sources is often inconsistent, unpredictable, and unevenly distributed due to the geographical separation of energy production and consumption areas. This makes it challenging to meet global energy needs, necessitating the creation of a new, more adaptable energy supply and demand system (Møller et al., 2017). Among the available options, hydrogen is an exceptionally efficient energy carrier due to its high gravimetric energy storage density of 120 MJ/kg (based on lower heating value) and its carbon-free nature during energy conversion. However, gaseous hydrogen has a much lower volumetric energy density of 9.8 kJ/L at standard temperature and pressure (STP) compared to conventional fossil fuels, which have energy densities of 31.7 MJ/L for gasoline and 15.8 MJ/L for methanol at STP. This low energy density makes it challenging to use it as a long-distance energy carrier, as transporting large volumes of gaseous hydrogen is currently not economically viable (Mazloomi and Gomes, 2012). Hydrogen (H_2) can be converted into alternative compounds known as energy vectors to address these challenges, which enable safe storage and transportation. These vectors can later be regenerated through thermal decomposition or endothermic reforming for on-site use (Tan et al., 2023). Potential energy vectors include chemical hydrides, formic acid, methanol, methylcyclohexane, liquid organic hydrides, and ammonia (NH_3), which all offer viable options for hydrogen storage in easily transportable liquid forms (Bay et al., 2023). Among the various methods available, ammonia has a remarkably high hydrogen mass storage capacity of 121 kg H_2/m^3 (Lamb et al., 2019) and is carbon-free during usage (Yapicioglu and Dincer, 2019). The IEA suggests that importing hydrogen in the form of ammonia could be more cost-effective in some regions than producing it domestically (Global Energy Review, 2025). Similarly, the Committee on Climate Change notes that converting hydrogen into ammonia for long-distance transport may offer lower costs than transporting hydrogen directly (Wijayanta et al., 2019). Ammonia has been manufactured in vast quantities for over 75 y, primarily as fertilizer.

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Its long-standing role in the industry has led to the development of a substantial storage and distribution network, backed by well-established regulations and a proven safety record (Abraham and Al-Mohannadi, 2022). Furthermore, ammonia can be readily liquefied at -33.15 °C under atmospheric pressure or through compression to 9.9 bar at room temperature and can be mass-produced through the well-established and commercialized Haber-Bosch (HB) process (Afif et al., 2016). While the HB process currently requires substantial energy and emits CO_2, efforts are underway to make this process more sustainable by integrating water electrolysis powered by renewable energy (Smith et al., 2020). Irrespective of the hydrogen feedstock source, once ammonia has been synthesized and transported to or near the site of utilization, it must undergo decomposition into nitrogen and hydrogen (Lamb et al., 2019). Subsequently, hydrogen must be separated and purified to conform to the composition standards established by the International Organization for Standardization (ISO) for fuel cells, specifically ISO 14687-2:2012 and 14687-3:2014 (Restelli et al., 2024).

Several techno-economic studies have assessed ammonia decomposition for hydrogen production, with reported costs varying depending on plant scale and system configuration. However, many of these studies do not account for hydrogen compression to high pressures, which is a crucial step for applications like Hydrogen Refueling Stations (HRS) that require hydrogen delivery at up to 350 bar for Fuel Cell Electric Vehicles (FCEVs) (Restelli et al., 2024). Moreover, reactor simulations in previous studies have often relied on equilibrium assumptions or simplified models, which may not accurately reflect catalytic performance under practical operating conditions. To address these gaps, the present study develops a fully integrated Aspen Plus® process model is developed, encompassing ammonia decomposition, hydrogen purification, and multistage compression up to 350 bar. The ammonia cracker is simulated using a kinetic model, and the system is designed for a production capacity of 400 kg H_2/d, consistent with recommended HRS capacities for urban mobility applications, as outlined in national policy frameworks (Kelly and Zhou, 2022). In addition, the economic evaluation incorporates region-specific cost factors relevant to the Indian context, including the cost of compression. The decomposition process is further optimized through heat recovery integration, enhancing thermal efficiency and reducing external energy demand. The combined process simulation and techno-economic analysis (TEA) enable both technical optimization and financial evaluation, supporting the development of scalable and cost-effective hydrogen production solutions.

2. Methodology

This study employs a systematic approach to evaluate the feasibility of the process of ammonia decomposition for hydrogen production, consisting of process simulation and TEA. The ammonia decomposition process is modelled using Aspen Plus® (V12.1) software to produce high-purity hydrogen with a production capacity of 400 kg H_2/d at an operating pressure of 350 bar. TEA assesses the economic viability of the process by analyzing capital and operational costs. The process flowsheet is shown in Figure 1.

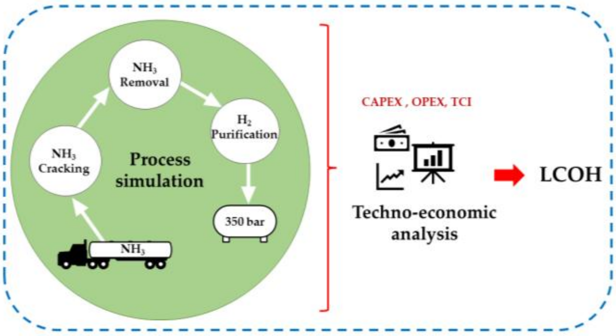

Figure 1: Flow diagram illustrating the research methodology

2.1 Ammonia Decomposition

The NH_3 decomposition reaction is temperature-dependent and endothermic, requiring thermal energy to break the stable NH_3 molecules into H_2 and N_2 (Motsa et al., 2024). The reaction of hydrogen production through ammonia decomposition can be represented by Eq(1) (Chen et al., 2021).

$$2NH_3 \rightleftharpoons N_2 + 3H_2 \quad (\Delta H_R^0 = 45.6 \text{ kJ mol } H_2^{-1}) \qquad (1)$$

Since the reaction is governed by equilibrium, a high temperature is needed for efficient NH_3 decomposition. The kinetics of the reaction play a crucial role in modeling the ammonia cracker, as they can significantly influence the size and cost of the equipment (Murmura and Annesini, 2021). A recent study suggests that the

Temkin-Phyzev equation accurately describes the kinetics of ammonia decomposition on Ruthenium-based catalysts under moderate temperatures and pressures, given in Eq(2) (Armenise et al., 2018).

$$r = k_0 e^{\left(\frac{-E_0}{RT}\right)} \left(\frac{{P_{NH_3}}^2}{{P_{H_2}}^3}\right)^{\beta} \tag{2}$$

where k_0 is a pre-exponential factor, E_0 is the activation energy, R is the universal gas constant, and T is the reaction temperature in Kelvin. The reaction rate is influenced by both ammonia and hydrogen pressures (P). The kinetic order of the NH_3 decomposition process is denoted by β. This model can effectively compare and fit with experimental data for the NH_3 decomposition reaction process.

2.2 Process Simulation

The process of ammonia decomposition was modelled using Aspen Plus® software to produce 400 kg H_2/d of hydrogen at 350 bar (Figure 2). The ammonia feed stream and air stream were preheated using a heat exchanger (MHeatX). The reaction kinetics were simulated using the RPLUG model, while the burner was simulated using the RGIBBS reactor. To support combustion, 18 % of the product gas was recycled as a fuel source. Heat from the high-temperature product stream is recovered using heat exchangers to preheat the ammonia feed and air stream. The product gas is then sent to the adsorption column, which removes unreacted ammonia. The purified N_2-H_2 stream is compressed to 15 bar before entering a Pressure Swing Adsorption (PSA) unit, where pure hydrogen will be separated (Grande and Rodrigues, 2005). A pseudo-PSA (black box) model built into Aspen Plus® was used, with 99 % hydrogen purity and 90 % recovery taken from literature (Barg et al., 2000). Finally, the hydrogen is compressed through a two-stage compressor to 350 bar (Restelli et al., 2024), that meets the pressure requirements for vehicle refueling.

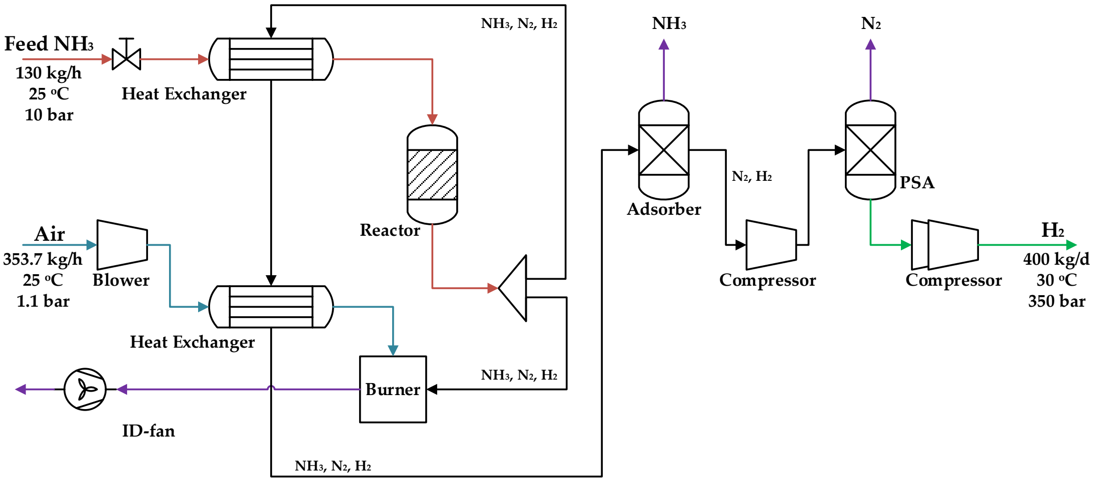

Figure 2: Ammonia Decomposition Process flowsheet

2.3 Economic Analysis

The economic evaluation of the ammonia decomposition plant includes CAPEX, OPEX, and annualized life cycle cost (ALCC) over its lifespan. The cost-driving processes were assessed using the Turton methodology (Turton et al., 2008), which provides a preliminary estimate of plant costs and serves as an initial feasibility study. The purchase base cost $C^0_{p,i}$, of equipment was calculated using Eq(3).

$$\log_{10}(C^0_{p,i}) = K_{1,i} + K_{2,i}\log_{10}(A_i) + K_{3,i}\,[\log_{10}(A_i)]^2 \tag{3}$$

where A_i is the capacity or size parameter, and value of the constants $K_{1,i}$, $K_{2,i}$ and $K_{3,i}$, specific to the type of equipment were obtained from (Turton et al., 2008). The equipment cost for the 2024 (y) was adjusted using the chemical engineering plant cost index (CEPCI) given in Eq(4) and scaled using Eq(5).

$$C_2 = C_1\left(\frac{I_2}{I_1}\right) \tag{4}$$

$$C_2 = C_1 \left(\frac{A_2}{A_1}\right)^n \tag{5}$$

where C_1 is the reference purchased equipment cost with size A_1 and cost index I_1 (CEPCI $_{2001}$ = 397), C_2 is the purchase cost estimated for this study with size A_2 and cost index I_2 (CEPCI $_{2024}$ = 798.8), and n is the cost exponent. The bare module cost $C_{BM,i}$, which accounts for the impact of equipment construction material and operating pressure, was estimated using Eq(6).

$$C_{BM,i} = C^0_{p,i} F_{BM,i} = C^0_{p,i}(B_{1,i} + B_{2,i} F_{M,i} F_{P,i}) \tag{6}$$

where $F_{BM,i}$ (the bare module factor) depends on two parameters: $F_{M,i}$ (the material factor), which is determined by the construction material and $F_{P,i}$ (the pressure factor), which reflects the operating pressure of the equipment. Constants $B_{1,i}$ and $B_{2,i}$, are specific to each type of equipment and can be obtained from (Turton et al., 2008). The total module cost includes an additional 18 % to account for contingency costs and administrative fees (Turton et al., 2008). The LCOH is the cost of producing hydrogen per unit mass, and it is essential to determine the CAPEX and OPEX to estimate it. ALCC was calculated using the cost recovery factor (CRF) and Fixed capital investment (FCI) or CAPEX. The CRF and CAPEX can be determined based on the discount rate (i), and plant lifespan (n), as outlined in Eq(7) and Eq(8), respectively. The LCOH has been calculated as Eq(9), and the key economic assumptions are listed in Table 1.

$$\mathrm{CRF} = \left(\frac{i(i+1)^n}{(i+1)^n - 1}\right) \tag{7}$$

$$\mathrm{ALCC} = \mathrm{CRF} \times \mathrm{CAPEX} \tag{8}$$

$$\mathrm{LCOH} = \frac{\mathrm{ALCC} + \mathrm{OPEX}}{\text{Anuual production capacity}} \tag{9}$$

Table 1: List of economic assumptions

Parameter	Value	Reference
Water cost, \$ / m^3	1	(Santana et al., 2024)
Electricity, \$ / MWh	80	(IEA, 2025)
Catalyst cost, \$ / kg	24	(Devkota et al., 2024)
Discount rate, %	10	(Devkota et al., 2024)
Plant life, y	20	(El-Shafie et al., 2024)
Labour cost, \$/y (4 per shift; 3 operators,1 manager)	109,756	(El-Shafie et al., 2024)
Maintenance	3 % of FCI	(Turton et al., 2008)
Insurance	1.5 % of FCI	(Turton et al., 2008)

3. Results and Discussion

The process employed heat recovery from the product stream through a heat exchanger unit to preheat the feed and air streams to 300 °C and 347 °C, respectively. The product stream has a composition of 74.5 % N_2, 24.8 % H_2 and 0.45 % NH_3. The decomposition of ammonia as a function of the reactor length is shown in Figure 3a. The simulation of the ammonia decomposition unit results in 99 % conversion efficiency with a 470 °C reactor outlet temperature. The product gas was subsequently cooled through a heat exchanger to meet the required temperature for the adsorption column, facilitating the removal of unreacted ammonia while recovering heat to preheat the feed and air streams. The product gas was then passed to the pressure adsorption column (PSA) to obtain 99 % pure hydrogen gas, which was compressed to 350 bar using a multistage compressor. The 400 kg/d production capacity is sufficient to fuel approximately 70 FCEVs daily.

The CAPEX of the ammonia decomposition plant with 400 kg/d of hydrogen production at 350 bar was estimated to be \$ 712,000. The compressor cost accounts for 44 % of the overall capital investment, while the ammonia cracker accounts for 21 %, as shown in Figure 3b. The cost of manufacturing (COM) or OPEX includes all expenses incurred during the plant operation, estimated to be \$ 898,000. The detailed breakdown of the CAPEX and OPEX for an ammonia cracking plant is provided in Table 2. The ammonia cost was the most significant contributor, followed by other costs associated with utilities, labour, maintenance, and insurance. The LCOH for producing 400 kg of H_2/d was estimated to be 6.57 \$ / kg. This value lies between the values reported in previous studies for ammonia decomposition systems at different scales. Makhloufi and Kezibri (2021) reported a CAPEX of $ 64,050,000 and LCOH of 4.83 $/kg for a large-scale plant producing 2 × 10^6 kg H_2/d. Devkota et al. (2024) estimated LCOH 6.05 $/kg for 11,153 kg H_2/d and a CAPEX of $ 2,130,00, while Restelli et al. (2024) reported 7.51 $/kg for a decentralized 500 kg H_2/d plant, with a CAPEX OF $ 54,000. However, these studies did not include hydrogen compression costs for refueling applications. When compared with other green hydrogen production pathways, large-scale electrolysis systems have reported LCOH values of 5.29 $/kg for alkaline and 5.92 $/kg for PEM configurations at a 100 MW scale, based on electricity prices of 60 $/MWh (Pinheiro et al., 2025). In contrast, the present ammonia-based system, with a production capacity of 400 kg H_2/d and integrated compression to 350 bar, offers a competitive and practical solution for decentralized hydrogen supply.

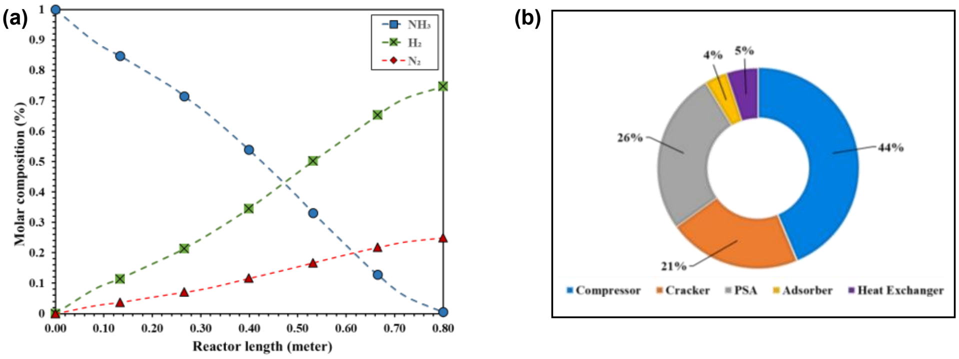

Figure 3: (a) Molar composition vs the reactor length, (b) Percentage distribution of equipment cost.

Table 2: The estimated cost breakdown of a 400 kg H_2/d ammonia cracking plant

Components	Cost ($/y)
Direct costs	
Equipment cost	520,123
Installation, piping, and buildings	98,472
Indirect cost	93,622
Total capital investment (CAPEX)	712,218
Annualized life cycle cost (ALCC)	83,329
Direct production costs	
Raw material, utilities	615,605
Maintenance	21,366
Labour	109,728
Fixed charges, taxes, and insurance	10,683
Total operating expenditure (OPEX)	898,124
LCOH ($/kg H_2)	6.57

4. Conclusion

This study evaluates the techno-economic feasibility of hydrogen production through catalytic ammonia decomposition. The process achieves 99 % ammonia conversion efficiency at a reactor outlet temperature of 470 °C. The proposed 400 kg/d system has a CAPEX of $ 712,000 and an OPEX of $ 898,000, leading to an LCOH of 6.57 $/kg. The economic analysis further indicates that this approach is cost-competitive with alternative hydrogen production technologies, particularly when the compression requirements for end-use applications are considered. Future work should explore the integration of green ammonia produced from renewable sources, enabling a fully carbon-neutral supply chain. Comparative assessments with conventional green hydrogen pathways, such as electrolysis, would further clarify the most sustainable and economically viable options for large-scale deployment.

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