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REVIEW ARTICLE

# Green ammonia: catalysis, combustion and utilization strategies

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## Abstract

Engineering is about observing physical conditions and being able to mathematically model the systems and solve problems for optimal design parameters using well-defined mathematical approaches. The government of India's creation of a market for green hydrogen and ammonia promotes the development of newer technologies for producing and using these green fuels. One of the most popular processes for manufacturing ammonia is the Haber-Bosch process of 1904, which needs a high temperature of around 500°F and a high pressure of 150 to 300 bar. A study on the synthesis of green ammonia from nitrogen and water using renewable energy sources like sun and wind was discovered for the first time in 2013. Start-ups worldwide are developing a tabletop hydrogen generator technology that breaks ammonia and creates high-grade hydrogen suitable for fuel cells.

**Keywords**: Ammonia combustion, Ammonia synthesis reactor, Ammonia Utilization, Electr-chemical ammonia synthesis, Fuel cells, Green ammonia, Green fuels, Green hydrogen, Renewable Energy, Thermo-chemical ammonia synthesis.

## Introduction

The National Hydrogen Mission of India, which was announced on August 15, 2021, is assisting the country in becoming a global powerhouse for hydrogen technologies and production. According to research by the International Environmental Agency (IEA), the government would create demand and market for hydrogen technology in specific areas such as fertilizers, steel, and petrochemical industries, as well as clean hydrogen demonstrations in the transportation sector. The Indian government has allocated 1500 million rupees in the 2021-22 budget to boost renewable energy technologies in order to reach the objective of 175 kW of renewable energy capacity by 2022 (IEA/ IRENA Renewable Policies Database, 2022). Protocols and summits worldwide emphasize the importance of limiting global warming to less than 2°C. Transitioning to green hydrogen and green ammonia is one of the most important needs for reducing emissions, especially in hard-to-abate sectors - any area where the shift is difficult or impossible due to a lack of technology or a high cost (Green Hydrogen Policy, 2022). According to the Green Hydrogen Policy, "Green Hydrogen" or "Green Ammonia" refers to hydrogen or ammonia created by electrolyzing water using renewable energy (2022). Interstate energy transmission fees for the production of green hydrogen/green ammonia projects commissioned before June 30, 2025 are waived, according to a study from the Ammonia Energy Association (Atchison, 2022).

Figure 1 depicts how basic energy resources are used in different countries. Over the last two decades, India's energy consumption has continuously climbed. From a health standpoint, this constant growth in energy consumption from mostly carbon sources is concerning; thus, it is critical to become carbon-free. In light of these developments, a thorough understanding of the synthesis mechanism of green fuels such as hydrogen/ammonia and the most recent trends in reaction catalysis in ammonia generation is required. Furthermore, in the development of near-future renewable energy systems (RES) for both stationary and

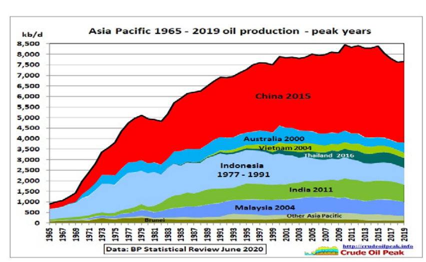


**Figure 1:** Primary Energy Consumption

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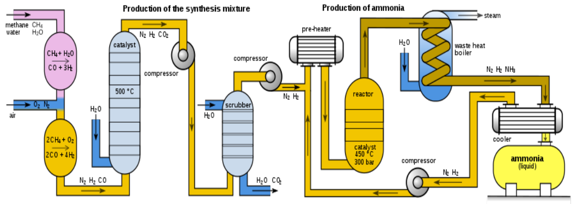


**Figure 2:** Process Flow Diagram (Haber Bosch Process)

mobile applications, the optimal design of catalytic reactors and the combustion characteristics of these green fuels are important factors to address.

### *Traditional Ammonia Synthesis*

The government of India's creation of a market for green hydrogen and ammonia promotes the development of newer technologies for producing and using these green fuels. Because the direct use of solar, wind, and tidal energy suffers from intermittency, ammonia is seen as a crucial energy vector and carrier to lead the de-carbonization theme throughout countries (Elbaz *et al.*, 2022). One of the most popular processes for manufacturing ammonia is the Haber-Bosch process of 1904, which needs a high temperature of around 500°C and a high pressure of 150 to 300 bar. The high prices, energy consumption, and excessive $CO_2$ emissions force researchers to create new approaches incorporating a simpler ammonia production process under mild conditions.

Haber Bosch's process flow diagram is shown in Figure 2. The process employs ambient air, methane, and water at the inlet. After $CO_2$ removal, the steam is reformed and pure gases are passed to the catalyst bed. The gases recombine at the right conditions, and ammonia synthesis is formulated. To describe the stoichiometry and flow physics, new CFD approaches are being investigated.

Kordali *et al.* (2000) produced ammonia at 20°C from di-nitrogen and water using a Ru/C cathode and Pt anode with 2 mol KOH aqueous solution as electrolyte and a Nafion Membrane as separation membrane, reporting an ammonia synthesis rate of 170 ng $h^{-1}$ $cm^{-2}$ (Kordali, Kyriacou, & Lambrou, 2000). Some developed plants were able to directly generate ammonia and its derivatives from air and water accessible at normal atmospheric conditions, according to Burns and Hardy (Burns & Hardy, 1975). For the first time, Lan R *et al.* reported on the manufacture of Green Ammonia from nitrogen and water utilizing renewable energy sources such as solar and wind (Lan, Irvine, & Tao, 2013). A voltage of 1.6 V resulted in a maximum ammonia production rate of 1.14 $10^{-5}$ mol $m^{-2}$ $s^{-1}$. Under favorable conditions, this might offer a different route for the widespread synthesis of the fundamental chemical ammonia.

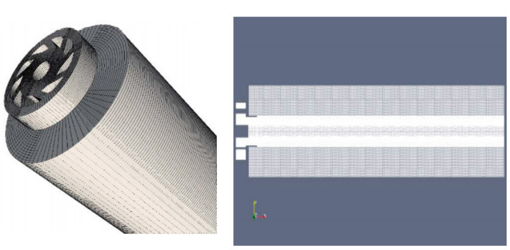

**Figure 3:** Meshing of Swirl Combustion Chamber (Xiao *et al.*, 2017)

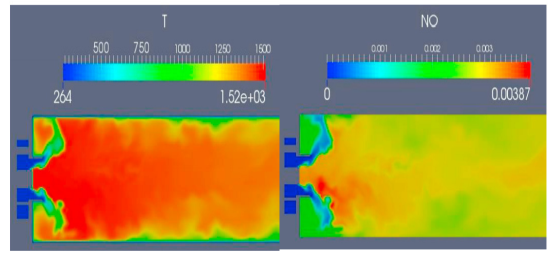


**Figure 4:** Temperature Profile in the Combustion Chamber (Xiao et al., 2017)

### *Computational Approaches in Ammonia Combustion*

Engineering is about observing physical conditions and being able to mathematically model the systems and solve problems for optimal design parameters using well-defined mathematical approaches. Md. Burhan Kabir Suhan *et al.* created a steady state 1 - D model for an axial flow industrial catalytic bed ammonia converter (Suhan *et al.*, 2022). Mathematical solvers have gained widespread acceptance, as seen by the large number of articles utilizing computational techniques.

For the simulation of this combustion chamber, Xiao *et al.* (2017) created a structured mesh with 0.8 million cells, as shown in Figure 3. Local meshing and refinement in specific areas of the mesh is used to capture the turbulent behavior of flames and reaction chemistry.

Because renewable energy sources are highly unreliable, a mature energy carrier such as pure hydrogen/ammonia is offered as a near-term alternative. Direct burning of ammonia through gas turbines is considered a sustainable alternative to typical fossil fuel utilization in big industrial applications. A Computational Fluid Dynamics (CFD) program with chemistry modules gives you more options for understanding the mechanics of combustion flow inside gas turbines. Using a Large Eddy Simulation Model with turbulence coupled equations, Xiao *et al.* (2017). reported the characteristics of the flow field, including pressure, velocity, re-circulation behavior, flame structure, and emissions with a premixed lean mixture of ammonia and hydrogen in a generic swirl burner in 2017.

The temperature profile inside the combustion zone for the premixed lean mixture steady-state combustion analysis and the NO generation in the fluid domain are depicted in Figure 4. Xiao *et al.* (2017) found a good correlation between the simulation and the experiments conducted in a gas turbine facility at Cardiff University in the United Kingdom.

**Table 1:** Life cycle cost of hydrogen production

| *Scale of hydrogen production (cu.m/hr)* | *Cost of hydrogen production (US Dollars)* | | | |
|---|---|---|---|---|
| | *Water electrolysis* | *Natural gas reformation* | *Methanol reformation* | *Ammonia cracking* |
| 10 | 0.943 | 0.390 | 0.380 | 0.343 |
| 100 | 0.814 | 0.261 | 0.285 | 0.279 |
| 1000 | 0.739 | 0.186 | 0.226 | 0.241 |

In line with these ammonia research techniques, a separate team of scientists is investigating the potential thermal cracking of ammonia at high temperatures and pressures to produce hydrogen from renewable sources.

### *Ammonia - Hydrogen Conversion for Pemfc Applications*

Given the inherent $NO_x$ emission difficulties associated with ammonia combustion, the feasibility of liquid ammonia operating as an energy carrier in hydrogen synthesis (since hydrogen in the gas phase takes up more volume) is now being investigated. Under 1 MPa at 298 K, liquid ammonia can hold around 10.7 kg of $H_2$ per 100 litres (Miyaoka, Ichikawa and Kojima, 2013). In thermal cracking operations, the removal of ammonia via absorption at ambient temperature promotes the removal of additional carbon sources. On the other hand, concentrated solar technologies are being employed to aid with separation. Rencat (Brown, 2017), a Danish start-up, is currently developing a tabletop hydrogen generator technology that breaks ammonia and creates high-grade hydrogen suitable for fuel cells. Figure 5 depicts recent research in Denmark aimed at lowering catalyst costs by switching from Ru/C-based catalysts to a low-cost Fe-Ni Alloy-based catalyst in the Selective Ammonia Oxidation (SAO) zone to produce PEMFC-grade hydrogen.

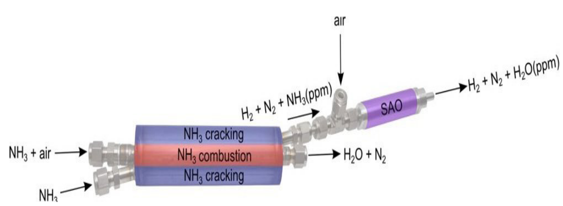


**Figure 5:** Selective Ammonia Oxidation (SAO) from a patent-pending catalyst, Rencat[#]

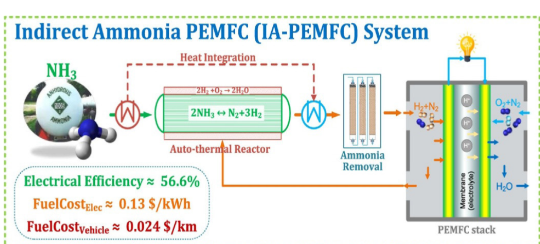


**Figure 6:** Schematic Layout of IA - PEMFC System

A mathematical model for an indirect ammonia polymer electrolyte membrane fuel cell (IA - PEMFC) system has been developed by Li Lin *et al.* Heat engines and direct H2 PEMFC applications were found to be less efficient than the system. The schematic layout of an IA-PEMFC is shown in Figure 6. It's worth noting that the system's electrical efficiency is expected to be 56.6% for an optimal heat integration configuration. The production of a unit (kWh) costs 0.13 dollars, while a unit (km) travel distance costs 0.024 dollars (Lin *et al.*, 2022).

Ammonia decomposition gas as a fuel is a similar line of thought related to fuel cell use. Using a mixed gas instead of pure hydrogen resulted in a 47% reduction in efficiency, according to Zhao *et al.* (2022). Once the hydrogen molar concentration falls below 0.12, the local current density reduces dramatically.

The life cycle cost of hydrogen production from several techniques outlined in a research text available at Intech open proposes the following: Table 1 depicts that thermal cracking of ammonia is the most common means of production for FC applications as well from an economic perspective.

Clear strategies are formed to promote hydrogen as a nationwide fuel in the near future, in accordance with Indian government policies and accompanying programs developed under MNRE.

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