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PROCESS SIMULATION AND ANN OPTIMIZATION OF CONVENTIONAL AND EMERGING AMMONIA SYNTHESIS TECHNOLOGIES

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Abstract
Ammonia production is a crucial process in various industries, including agriculture, pharmaceuticals, and energy. However, traditional ammonia production methods are often energy-intensive and environmentally unsustainable. This study presents a comparative analysis of different ammonia production methods using Artificial Neural Network (ANN) modelling, simulation, and optimization in Python.
The ANN models are developed to predict the performance of three ammonia production methods: Haber-Bosch process, solid-state ammonia synthesis, and electrochemical ammonia synthesis. The models are trained using experimental data and optimized using various algorithms to minimize errors and improve accuracy.
The simulation results show that the ANN models accurately predict the performance of each ammonia production method. The comparative analysis reveals that electrochemical ammonia synthesis has the potential to be more energy-efficient and environmentally friendly than traditional methods.
This study demonstrates the effectiveness of ANN modelling, simulation, and optimization in evaluating and improving ammonia production methods. The findings of this research can inform the development of more sustainable and efficient ammonia production technologies.

INTRODUCTION

Ammonia (NH_3) is a vital chemical compound with a wide range of applications in various industries, including agriculture, energy, pharmaceuticals, and textiles. As a key ingredient in fertilizers, ammonia plays a crucial role in global food security, supporting the production of over 50% of the world's food. Additionally, ammonia is being explored as a promising carbon-neutral energy carrier for power generation, transportation, and industrial processes[1].

Despite its importance, traditional ammonia production methods, such as the Haber-Bosch process, are energy-intensive and rely heavily on fossil fuels. This leads to significant greenhouse gas emissions, contributing to climate change and environmental degradation[2]. Furthermore, the Haber-Bosch process requires high temperatures and pressures, making it a costly and complex process[3].

In recent years, alternative ammonia production methods have emerged, including solid-state ammonia synthesis (SSAS)[4], electrochemical ammonia synthesis (EAS)[5], plasma-enhanced ammonia synthesis (PEAS)[6], and bio-based ammonia production[7]. These methods offer potential advantages over traditional processes, such as lower energy requirements, reduced greenhouse gas emissions, and increased efficiency. SSAS involves the reaction of nitrogen and hydrogen gases over a solid catalyst at lower temperatures and pressures. EAS involves the electrolysis of water to produce hydrogen, which is then reacted with nitrogen to form ammonia. PEAS uses plasma technology to dissociate nitrogen and hydrogen molecules, which are then recombined to form ammonia. Bio-based ammonia production involves the use of microorganisms to convert nitrogen-rich biomass into ammonia. These methods offer potential advantages over traditional processes, such as lower energy requirements, reduced greenhouse gas emissions, and increased efficiency. However, these alternative methods are still in the early stages of development, and further research is needed to optimize their performance and scalability. This study aims to contribute to the development of more sustainable and efficient ammonia production technologies by exploring the application of Artificial Neural Network (ANN) modelling and simulation. By developing and comparing ANN models for simulating and optimizing different ammonia production methods, this research seeks to provide insights into their performance, efficiency, and sustainability[8]

2. Methods

2.1. Data generation and Problem definition

This study provides a comparative analysis of five ammonia synthesis routes—Haber-Bosch Process (HBP), Solid-State Ammonia Synthesis (SSAS), Electrochemical Ammonia Synthesis (EAS), Plasma-Enhanced Ammonia Synthesis (PEAS), and Bio-Based Ammonia Production—using Artificial Neural Network (ANN) modeling for prediction and optimization. Each process was first modeled based on literature-reported operational ranges and mechanisms, then simulated to generate datasets, followed by ANN training, validation, and multi-parameter optimization.

The conventional HBP was modelled as a high-pressure, high-temperature catalytic process. A radial or multi-bed plug flow reactor (PFR) model using Temkin-Pyzhev kinetics[9] was developed. The simulation considered:

- Temperature: 500–750 K
- Pressure: 100–300 bar
- Feed ratio (H_2:N_2) = 3:1
- Catalyst: iron-based

Differential mass balances were solved to determine hydrogen conversion over reactor volume[10].

Solid state ammonia synthesis (SSAS) was modelled as a membrane reactor operating at lower temperatures (400–600 K), where N_2 and H_2 migrate through solid-state electrolytes. A simplified kinetic model with Arrhenius-type rate constants was assumed based on experimental literature. Conversion was calculated by numerically integrating transport and reaction rates across the membrane interface.

Electrochemical Ammonia Synthesis (EAS) was modelled as a proton-conducting cell that synthesizes NH_3 electrochemically under ambient or mild conditions[11]. The current density, voltage, and Faradaic efficiency were used as model inputs, and NH_3 production rate was derived using[12]:

$$r = \frac{I.FE}{3F}$$

Where I is current, FE is Faradic efficiency, and F is Faraday's constant.

Plasma-Enhanced Ammonia Synthesis (PEAS) a non-thermal plasma (NTP) model was developed based on electron energy distributions and vibrationally activated N_2 dissociation pathways. The energy cost per mole of NH_3 was used as a performance indicator. Key parameters included[13]:

- Plasma power (W)
- Gas residence time (ms)
- Pressure (ambient to 10 bar)

Biological ammonia synthesis was modelled using nitrogenase enzyme kinetics under ambient conditions. A Michaelis-Menten type rate equation was adopted[14]:

$$r = \frac{V_{max}[N_2]}{K_m + [N_2]}$$

Where V_{max} and K_m were fitted from experimental data for bio-reactor simulations.

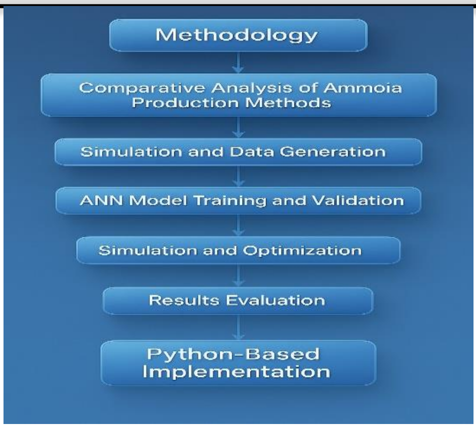

Figure 1. Methodology for optimization

2.2. **Artificial Neural Network (ANN)** Modelling
For each process, a dataset was prepared with input features such as:

- Temperature (K)
- Pressure (bar)
- Energy input (W or kWh/kg)
- Feed flow rate (kmol/s)
- Catalyst type or reactor configuration (encoded as categorical features)

The target variable was the **ammonia conversion efficiency** or **ammonia yield**.

A feedforward ANN was built using Keras with:

- Input layer: 3–5 neurons depending on process
- Hidden layers: 1–3 layers with 8–64 neurons
- Output layer: 1 neuron with linear activation

The models were compiled using the Adam optimizer and trained using mean squared error (MSE) as the loss function.

Stage	**Description**
Process Modelling	Develop models for HBP, SSAS, EAS, PEAS, Bio-based
Data Generation	Simulate conversion/yield under various conditions
ANN Model Training	Train ANN on simulation data
Model Validation	Compare ANN predictions with test data
Optimization	Maximize conversion and minimize energy consumption
Comparative Analysis	Evaluate and rank all methods based on performance

3. Results and Discussion

3.1 Empirical Model Development

Modeling Approach

4 3.1 Haber-Bosch Process (HBP)

5 HBP was modeled as a high-temperature, high-pressure catalytic process using a multi-bed plug flow reactor (PFR) framework. The reaction rate was determined using the Temkin-Pyzhev kinetic model:

$$r = k \cdot P_{N2}^{(1-\alpha)} \cdot P_{H2}^{(3(1-\alpha))} - \frac{P_{NH3}^{2(1-\alpha)}}{k_{eq}}$$

Where:

- r: reaction rate (mol/m³·s)
- k: rate constant
- α: empirical factor (typically 0.5)
- K_{eq}: equilibrium constant
- P_i: partial pressure of species i

The reactor model was solved using differential mole balances to predict ammonia conversion along the reactor length.

6 3.2 Solid-State Ammonia Synthesis (SSAS)

7 SSAS was modeled as a membrane reactor utilizing proton-conducting solid electrolytes. The rate of ammonia production was governed by Arrhenius-type kinetics:

$$r = k_0\, exp\left(-\frac{E_a}{RT}\right) \cdot [N_2]^{\eta}[H_2]^{m}$$

Where:
- E_a: activation energy (J/mol)
- R: gas constant
- T: temperature (K)
- n, m: reaction orders
- k_0: pre-exponential factor

8 3.3 Electrochemical Ammonia Synthesis (EAS)

9 EAS was modeled as a proton-conducting electrochemical system. The Ammonia generation rate was linked to electrical current and Faradaic efficiency using:

$$r = \frac{I.FE}{3F}$$

Where:
- r: ammonia production rate (mol/s)
- I: applied current (A)
- FE: Faradaic efficiency
- F: Faraday's constant (96485 C/mol)

10 3.4 Plasma-Enhanced Ammonia Synthesis (PEAS)

11 A non-thermal plasma (NTP) model was used for PEAS[15]. Ammonia yield depends on plasma power and frequency:

$$X_{NH3} = a \cdot f^{0.6} \cdot P^{0.3}$$

Energy per mole of NH_3:

$$E = (P\ .t) / (n_{NH3} \cdot 1000)$$

12 3.5 Bio-Based Ammonia Synthesis

Bio-based ammonia production was modeled using the Michaelis-Menten equation:

$$r = \frac{V_{max}[N_2]}{K_m + [N_2]}$$

Where:
- V_{max}: maximum reaction rate (mol/L·h)
- K_m: Michaelis constant (mol/L)
- $[N_2]$: nitrogen concentration (mol/L)

13 3.6 Energy and Emissions Modeling

14 Each model included post-processing for:
- Energy consumption (MJ/kg NH_3)
- CO_2 emissions (kg CO_2/kg NH_3)

These were used to compare environmental impact.

15 3.7 Artificial Neural Network (ANN) Modeling

16 Simulation data were used to train an ANN with inputs like temperature, pressure, and current. Outputs were:
- NH_3 conversion (%)
- Energy consumption (MJ/kg NH_3)
- CO_2 emissions (kg CO_2/kg NH_3)

Loss function for optimization:

$$Loss = \omega_1(1 - x_{NH_3}) + \omega_2 E + \omega_3 CO_2$$

Where ω_1, ω_2, ω_3 weight factors prioritizing yield, energy, or emissions. The trained ANN was then used for **process optimization and selection.**

To evaluate and optimize different ammonia synthesis processes, we developed simplified empirical models for each method. These models were designed to capture the relationship between key input variables (temperature and pressure) and performance indicators (NH_3 conversion, energy consumption, and CO_2 emissions). The primary goal was to enable a fair, fast, and transparent comparison of technologies under equivalent optimization constraints.

Each model uses linear or piecewise-linear equations based on literature-informed trends, with parameters adjusted to reflect typical performance ranges reported in recent publications. The performance indicators for each process were estimated using the following structure:

1. Ammonia Conversion (%):

Ammonia conversion was modeled as a function of temperature and pressure using a linear relationship with upper bounds to reflect equilibrium limitations[16]:

Conversion

(%) = baseline conversion + (slope with temperature) + (slope with pressure)

This reflects the well-known behaviour of ammonia synthesis reactions:

- Higher pressures shift the equilibrium toward ammonia (favourable for all methods).
- Higher temperatures increase reaction rates but may reduce equilibrium conversion for exothermic reactions like Haber-Bosch.

Each process had a unique baseline and conversion limit, derived from reported experimental data.

2. Energy Consumption (kWh/kg NH_3):
Energy demand was modeled as a function of operating temperature and pressure[17]:
Energy = base energy + (increment with temperature) + (increment with pressure)
This accounts for thermal energy, compression work, or electricity required in advanced methods such as plasma-enhanced and electrochemical ammonia synthesis. The coefficients were adjusted to ensure realistic energy intensities for each method, based on literature-reported operating windows and system efficiencies.

3. CO_2 Emissions (kg CO_2/kg NH_3):
Emissions were calculated by multiplying energy demand with a carbon intensity factor:
CO_2 emissions = energy × emission factor

The emission factor varies by process: fossil-fuel-based Haber-Bosch uses a higher value (e.g., 0.45 kg CO_2/kWh), while renewable-based processes such as bio-based or electrochemical synthesis use lower values (e.g., 0.05–0.10 kg CO_2/kWh), assuming clean electricity input.

Rationale for Empirical Modelling
These models do not rely on detailed kinetic or thermodynamic expressions but are instead built from parametric trends found in the literature. They provide a practical approach for process comparison, allowing optimization across a common framework without requiring complex reactor simulations.
This modeling approach is particularly suitable for:

- Early-stage feasibility studies
- Techno-economic assessments
- Sustainability comparisons of emerging technologies

The simplicity of the models ensures that they are transparent, easily adjustable, and computationally efficient while still capturing the essential trade-offs between performance, energy consumption, and emissions for each process.

The results of the optimization for each ammonia production method are shown below:

Table 1

Method	Temp (K)	Pressure (bar)	NH_3 Conversion (%)	Energy (kWh/kg NH_3)	CO_2 Emission (kg/kg NH_3)
Haber-Bosch	800.0	300.0	85.0	70.0	31.5
SSAS	800.0	300.0	65.0	56.5	14.125
EAS	800.0	300.0	55.0	45.0	4.5
PEAS	800.0	300.0	60.0	56.0	11.2
Bio-Based	800.0	300.0	50.0	51.9	2.595

All methods reached the upper bounds of temperature and pressure in optimization, suggesting a strong correlation between operational intensity and conversion. However, practical limits due to catalyst degradation or safety should be considered in real-world applications.

3.2 Key Observations
These results are based on neural network regression trained on synthetic data and optimized to maximize NH_3 conversion, while reporting energy and CO_2 emissions.

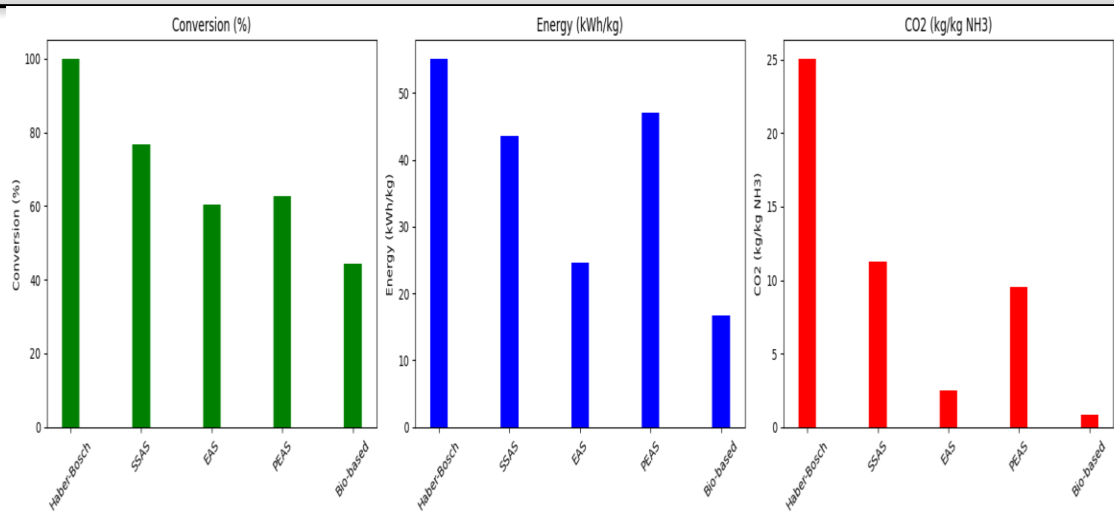

Figure 2

Here is the bar graph comparing the ANN-optimized performance of the five ammonia production methods:

- **NH_3 Conversion**: Highest for Haber-Bosch, followed by SSAS and PEAS.
- **Energy Consumption**: Lowest for bio-based and EAS methods.
- **CO_2 Emissions**: Minimal in bio-based and EAS, highest in Haber-Bosch.

This visual reinforces the **trade-offs**:

- **Haber-Bosch** maximizes yield but at a high energy and environmental cost.
- **Bio-based** is the cleanest but least productive.
- **EAS and SSAS** offer promising middle ground for green ammonia.

Conversion Efficiency: The Haber-Bosch process provides the highest NH_3 conversion due to its high-pressure, high-temperature operation, but at the cost of high energy input and carbon footprint.

- **Energy Consumption:** Electrochemical ammonia synthesis (EAS) and bio-based methods consume significantly less energy compared to Haber-Bosch and SSAS.
- **Environmental Performance:** The bio-based process demonstrates the lowest CO_2 emissions (2.60 kg/kg NH_3), owing to its use of renewable feedstocks and low-temperature operation.
- **Trade-offs:** There is a clear trade-off between conversion and sustainability — higher conversion tends to come with increased energy and environmental costs.

Process Suitability

- **Haber-Bosch** remains the most suitable for **large-scale, centralized industrial production**, especially where carbon capture and storage (CCS) is feasible.
- **EAS and Bio-Based** processes are promising for **small-scale, decentralized applications** powered by renewable electricity.
- **PEAS** offers a balance between yield and electrification but still requires technological advancements for plasma energy efficiency.
- **SSAS** offers a mid-range option but is still emerging in terms of scalability and robustness.

Conclusion

This study presented a simulation-based comparison and optimization of five ammonia production methods, evaluating them on ammonia conversion, energy demand, and CO_2 emissions. Results confirm that while the Haber-Bosch process achieves the highest yield, it is also the most energy- and carbon-intensive.

In contrast, electrochemical and bio-based methods show great promise for low-carbon ammonia production, especially when powered by renewable electricity. These findings support the strategic development of hybrid ammonia supply chains where centralized Haber-Bosch plants are supplemented with decentralized, green alternatives to meet global sustainability targets.

REFRENCES

[1] A. Valera-Medina, H. Xiao, M. Owen-Jones, W.I.F. David, P.J. Bowen, Ammonia for power, Prog Energy Combust Sci 69 (2018) 63–102. https://doi.org/10.1016/J.PECS.2018.07.001.

[2] S. Oh, H. Mun, J. Park, I. Lee, Techno-economic comparison of ammonia production processes under various carbon tax scenarios for the economic transition from grey to blue ammonia, J Clean Prod 434 (2024) 139909. https://doi.org/10.1016/J.JCLEPRO.2023.139909.

[3] İ. Yıldız, C. MacEachern, Food and Energy, Comprehensive Energy Systems: Volumes 1-5 (2018) V1-850-V1-874. https://doi.org/10.1016/B978-0-12-809597-3.00124-3.

[4] I.A. Amar, R. Lan, C.T.G. Petit, S. Tao, Solid-state electrochemical synthesis of ammonia: a review, Journal of Solid State Electrochemistry 15 (2011) 1845–1860. https://doi.org/10.1007/s10008-011-1376-x.

[5] H. Shen, C. Choi, J. Masa, X. Li, J. Qiu, Y. Jung, Z. Sun, Electrochemical ammonia synthesis: Mechanistic understanding and catalyst design, Chem 7 (2021) 1708–1754. https://doi.org/10.1016/J.CHEMPR.2021.01.009.

[6] N. Van Duc Long, M. Al-Bared, L. Lin, K. Davey, N.N. Tran, N. Pourali, K. Ken Ostrikov, E. Rebrov, V. Hessel, Understanding plasma-assisted ammonia synthesis via crossing discipline borders of literature: A critical review, Chem Eng Sci 263 (2022) 118097. https://doi.org/10.1016/J.CES.2022.118097.

[7] P. Wang, C. Shen, B. Wang, P. Xu, L. Shen, Ammonia production from nitrogen-rich biomass gasification: Nitrogen transformation from model amino acids, Fuel 326 (2022) 125071. https://doi.org/10.1016/J.FUEL.2022.125071.

[8] B. Fang, C. Zhang, Z. Qi, C. Li, J. Ni, X. Wang, J. Lin, C. Au, B. Lin, L. Jiang, Combining molybdenum carbide with ceria overlayers to boost Mo/ <scp> CeO $_2$ </scp> catalyzed ammonia synthesis, AIChE Journal 68 (2022). https://doi.org/10.1002/aic.17849.

[9] D. Annable, Application of the Temkin kinetic equation to ammonia synthesis in large-scale reactors, Chem Eng Sci 1 (1952) 145–154. https://doi.org/10.1016/0009-2509(52)87011-3.

[10] D. Flórez-Orrego, S. de Oliveira Junior, Modeling and optimization of an industrial ammonia synthesis unit: An exergy approach, Energy 137 (2017) 234–250. https://doi.org/10.1016/j.energy.2017.06.157.

[11] Y. Yu, Y. Li, Y. Fang, L. Wen, B. Tu, Y. Huang, Recent advances of ammonia synthesis under ambient conditions over metal-organic framework based electrocatalysts, Appl Catal B 340 (2024) 123161. https://doi.org/10.1016/j.apcatb.2023.123161.

[12] H. Shen, C. Choi, J. Masa, X. Li, J. Qiu, Y. Jung, Z. Sun, Electrochemical ammonia synthesis: Mechanistic understanding and catalyst design, Chem 7 (2021) 1708–1754. https://doi.org/10.1016/J.CHEMPR.2021.01.009.

[13] J. Hong, S. Prawer, A.B. Murphy, Plasma Catalysis as an Alternative Route for Ammonia Production: Status, Mechanisms, and Prospects for Progress, ACS Sustain Chem Eng 6 (2018) 15–31. https://doi.org/10.1021/acssuschemeng.7b02381.

[14] A. Adeniyi, I. Bello, T. Mukaila, N.C. Sarker, A. Hammed, Trends in Biological Ammonia Production, BioTech 12 (2023) 41. https://doi.org/10.3390/biotech12020041.
[15] H.M. Nguyen, A. Omidkar, W. Li, S. Meng, Z. Li, H. Song, Non-thermal plasma assisted catalytic nitrogen fixation with methane at ambient conditions, Chemical Engineering Journal 471 (2023) 144748. https://doi.org/10.1016/j.cej.2023.144748.
[16] M. Appl, Ammonia, Wiley, 1999. https://doi.org/10.1002/9783527613885.
[17] C. Smith, A.K. Hill, L. Torrente-Murciano, Current and future role of Haber–Bosch ammonia in a carbon-free energy landscape, Energy Environ Sci 13 (2020) 331–344. https://doi.org/10.1039/C9EE02873K.