



Indexing Green: A Financing Approach for Decarbonization of Ammonia

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Abstract

This study has two primary objectives. First, it reviews methods to reduce greenhouse gas (GHG) emissions in the ammonia industry. Second, it explores a policy intervention that could create an enabling environment for decarbonizing this sector. This policy mechanism is the use of green bonds to finance the industry's transition, with a particular emphasis on tokenized index-linked green bonds. These bonds feature coupon payments dynamically tied to the spot price of ammonia. Given their reliance on ammonia price fluctuations, accurately forecasting ammonia prices becomes an important sub-objective to structure these bonds effectively.

To achieve this, a Long Short-Term Memory (LSTM) network is employed to model and forecast ammonia prices. The analysis reveals a stable to modestly increasing price trend, which has significant implications for the performance of tokenized index-linked green bonds. Such bonds offer a base coupon rate plus a premium positively correlated with ammonia prices. As ammonia prices are projected to rise gradually over the forecast horizon, investors can expect increasing coupon payments, particularly during the bond's early lifecycle. This performance-linked structure incentivizes investment in decarbonization projects, aligning financial returns with environmental goals.

Decarbonization of the ammonia industry requires substantial capital investment in two main pathways. The first is blue ammonia production, where carbon capture, storage, and utilization (CCSU) technologies are integrated with the Haber-Bosch process to mitigate emissions. The second pathway involves producing green ammonia through water electrolysis to generate hydrogen, followed by applying the Haber-Bosch process to synthesize ammonia. Tokenized green bonds can be used to bridge the funding gap.

Keywords: Tokenization; Bonds; Decarbonization; Ammonia; LSTM

Introduction

In 2015, a new international treaty referred to as the Paris Agreement was agreed to by 196 countries to address the growing threat of climate change. The agreement aims to galvanize global efforts to limit global warming to well below 2°C above pre-industrial levels, with an aspirational target of capping the temperature rise at 1.5°C. To achieve this objective, each participating country is required to submit and implement its own action plan, referred to as Nationally Determined Contributions (NDCs) [1].

These NDCs are tailored to national contexts and outline specific commitments to reduce greenhouse gas (GHG) emissions across various sectors. Common high-emission sectors targeted in NDCs include heavy industry, electricity generation, transportation, agriculture, forestry, and waste management [2]. Among these, the heavy industry sector often encompasses the petrochemical industry, which in some nations includes the ammonia industry, which is a significant contributor to GHG emissions.

Ammonia (NH₃), a colorless gas with a sharp odor, is composed

of one nitrogen atom and three hydrogen atoms. It serves as an important input in multiple industries, including fertilizer manufacturing, industrial cleaning products, and refrigeration systems. Beyond its traditional uses, ammonia has also been identified as a potential long-term energy storage medium [3].

Ammonia is typically produced using feedstocks such as natural gas, coal, naphtha, or oil. Natural gas, primarily composed of methane (CH₄), is the most common feedstock used in ammonia production. This ammonia production process involves two key steps. The first is referred to as steam methane reforming (SMR). This is where methane is reacted with steam in the presence of a catalyst to produce a synthetic gas (syngas) (a mixture of hydrogen and carbon monoxide). The second step is the Haber-Bosch process, where purified hydrogen is combined with nitrogen to form ammonia [4]. While the SMR-Haber-Bosch is commercially feasible, the production of ammonia via this process generates substantial GHG emissions, with estimates ranging from 2.0 to 4.6 tons of carbon dioxide equivalent (CO₂e) per ton of ammonia, depending on plant efficiency [5].

To mitigate GHG emissions from ammonia production, countries are urging their industries to adopt alternative methods that modify traditional manufacturing processes. These approaches may include implementing carbon capture and storage (CCS), utilizing hybrid synthesis techniques, or adopting electrosynthesis for ammonia production. Despite these ambitions, many countries submitted their Intended Nationally Determined Contributions (INDCs) without clearly outlining the policies needed to achieve their stated goals. This gap is often bridged by framing NDCs as ‘conditional,’ meaning their implementation depends on receiving technical and financial assistance from the international community. In the absence of such support, these countries may fail to meet their targets. While the language of ‘conditional’ NDCs allows countries to avoid accountability for unmet goals, the reality of climate change persists, manifesting in escalating impacts such as more frequent and severe extreme weather events, rising sea levels, and ocean acidification [6]. Consequently, there is an urgent need for nations to take decisive action and fulfill their mitigation commitments under the Paris Agreement.

An energy storage medium or vector is a substance that acts as an intermediary for storing, transporting, and delivering energy from a source to an end user. Ammonia can serve as an energy storage vector by functioning as a medium for both storing and transporting energy [7].

This study has two key objectives. First, it aims to review the various methods available for reducing GHG emissions within the ammonia industry. Second, it seeks to consider policy interventions that could foster an enabling environment to drive the decarbonization of this industry. A particular policy mechanism is the use of green bonds to finance the industry’s transition. More specifically, tokenized index-linked green bonds where the coupon payments are dynamically tied to the spot price of ammonia. Given this financial instrument’s direct dependence on ammonia price fluctuations, a critical sub-objective emerges: developing accurate forecasts of ammonia’s spot price to properly structure these bonds.

The structure of the study is organized as follows. Section 2

delves into the widely used ammonia production process, the SMR-HB process. Section 3 examines alternative ammonia production techniques that have the potential to lower GHG emissions. Section 4 evaluates the policy tools that could drive GHG emission reduction initiatives in the ammonia industry. Section 5 provides a forecast of the ammonia prices. The corresponding methodology is placed in the Appendix. Finally, Section 6 provides the concluding remarks for this study.

2. Literature Review of Conventional Ammonia Production: Steam Methane Reforming and the Haber-Bosch Process (Grey Ammonia)

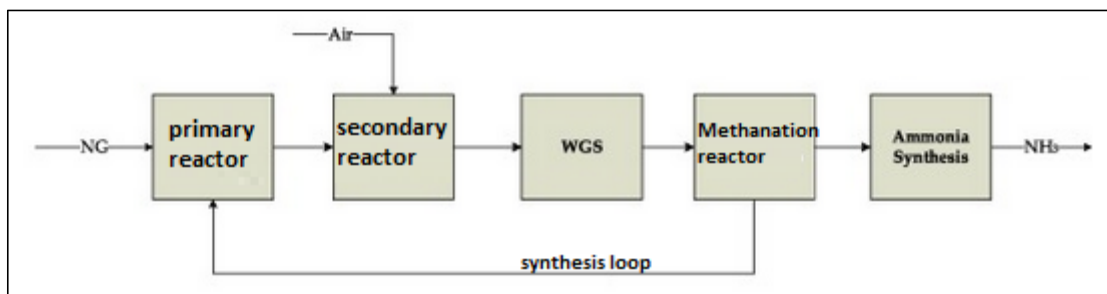
Ammonia production can utilize multiple feedstock sources, each requiring distinct processing methods. Coal can be used as a feedstock through coal gasification. Ammonia can be produced where there is the thermal decomposition of coal in an oxygen-limited environment, which generates syngas, consisting mainly of hydrogen and carbon monoxide. This syngas then undergoes the Haber-Bosch process, where nitrogen reacts with hydrogen under high pressure and temperature to produce ammonia [8].

Petroleum-derived naphtha can also be used as a feedstock to produce ammonia. Similar to natural gas steam reforming, this process for making ammonia from naphtha involves converting the naphtha into hydrogen-rich syngas, which subsequently feeds into the Haber-Bosch synthesis loop for ammonia production [9].

Heavy petroleum fractions can also be converted into ammonia through partial oxidation. This pathway uses controlled combustion with limited oxygen to produce syngas containing hydrogen, carbon monoxide, and nitrogen, which is then processed through the Haber-Bosch process [10].

Natural gas-derived methane remains the dominant feedstock for ammonia production globally. The steam methane reforming route offers better hydrogen yield and lower operational complexity compared to other hydrocarbon-based methods.

Figure 1 displays a simplified layout of the SMR-HB process.



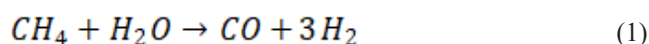
Source: Adapted from [11].

Figure 1: Ammonia Production through the SMR-HB Process

The first part of the process involves steam methane reforming. In the primary steam methane reforming (SMR) reactor, methane and steam undergo catalytic conversion at high temperatures (850–900°C) and pressures (25–35 bar). This endothermic reaction yields a mixture of hydrogen, carbon monoxide, residual methane, and steam. The required thermal energy is supplied by externally fired methane combustion within furnace tubes integrated with the catalyst bed.

The secondary reformer operates autothermally, combining partial oxidation with steam reforming. Compressed air is introduced to oxidize a portion of the methane-steam feedstock exothermically, maintaining temperatures of 900–1000°C without external heating. This self-sustaining reaction not only generates the required process heat but also introduces nitrogen, which is required for subsequent ammonia synthesis. Additionally, the SMR process co-produces steam, which can be recovered for downstream utilization.

The SMR process involves the following chemical reaction:



where CH_4 is the methane, H_2O is the steam from the water, CO is the carbon monoxide, and 3H_2 refers to three molecules of hydrogen.

The output from the secondary reactor consists of a mixture containing carbon monoxide, hydrogen, unreacted steam, and methane. This mixture is then directed to a two-stage water-gas shift (WGS) reactor, which aims to maximize the conversion of carbon monoxide into hydrogen. Within the WGS reactor, carbon monoxide reacts endothermically with steam to produce carbon dioxide and additional hydrogen. This step is important because hydrogen is the primary component required for ammonia synthesis.

Following the WGS reaction, carbon dioxide is removed from the gas stream. This is typically achieved using processes like the Benfield or Selexol methods, which employ solvents to selectively capture and separate carbon dioxide, leaving behind a purified hydrogen gas stream. Subsequently, a methanation reactor is utilized to minimize the risk of catalyst poisoning by converting any remaining carbon oxides into methane.

This means that the reactor can sustain its required operating temperature through the heat generated by the chemical reactions occurring within it, without the need for an external source providing continuous heating.

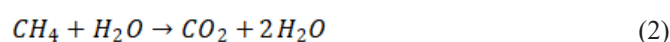
In the downstream synthesis loop, argon, an inert gas, and unreacted methane tends to accumulate over time. These components must be periodically purged to maintain the optimal composition and efficiency of the system.

During the ammonia production stage, the Haber-Bosch reactor facilitates the reaction between hydrogen and nitrogen to form ammonia. This reaction occurs under high-pressure conditions,

ranging from 15 to 25 megapascals (MPa), and elevated temperatures between 400°C and 450°C. An iron-based catalyst, such as magnetite or wustite, is used to accelerate the reaction rate.

However, only a small fraction of hydrogen and nitrogen reacts to form ammonia during a single pass through the reactor. To overcome this limitation and improve overall production efficiency, a gas recycling system is implemented. This system recirculates unreacted hydrogen, nitrogen, and other gases back into the reactor for additional passes. These repeated cycles significantly enhance the total conversion rate of the process.

Most of the carbon dioxide emissions in the SMR-HB process originate from the SMR stage. The combined reactions of SMR and the WGS process can be expressed as:



In this reaction, CO_2 refers to carbon dioxide, and 2H_2 represents two molecules of hydrogen. The release of CO_2 in these processes is primarily due to the carbon content of methane and its partial combustion during reforming.

To address this environmental concern, various approaches have been proposed to reduce CO_2 emissions associated with the SMR-HB process. These strategies are discussed in the following section.

Literature Review of Approaches for Reducing Carbon Dioxide Emissions Generated in Ammonia Production

The methods available for reducing carbon dioxide emissions in ammonia production can be categorized into two main approaches: i) the techniques that pairs the SMR-HB with carbon capture, storage, and use (CCSU); and ii) the techniques that involve the electrolysis of water [12-14].

Blue Ammonia Production (SMR-HB Paired with CCSU)

The pairing of the SMR-HB process with CCSU to mitigate carbon dioxide emissions is commonly referred to as blue ammonia production. In this approach, the carbon dioxide emitted during ammonia production is captured and transported via pipelines to either a geological formation for permanent storage or to a site where it can be utilized, such as in enhanced oil recovery operations [15].

Several methods exist for producing blue ammonia. Among the most prominent techniques are the Kellogg, Braun, and Root (KBR) process, the Linde Ammonia Concept (LAC), and the Gas Switching Reforming for Ammonia (GSR-NH3) process [17]. These processes are visually represented in Figure 2.

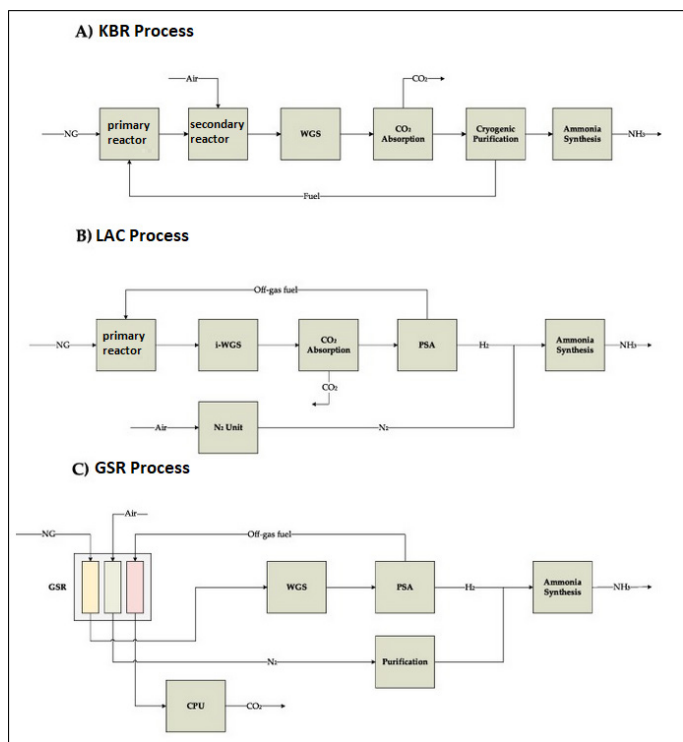


Figure 2: Different Blue Ammonia Processes (SMR-HB-CCSU)

The KBR process starts with methane being fed into a primary reactor, followed by a secondary reactor, to produce syngas. This syngas is composed of hydrogen, carbon monoxide, and a small amount of nitrogen from the air that remains unreacted during synthesis. To maximize hydrogen production, the WGS process is applied, and carbon dioxide is subsequently removed. Notably, the KBR process shares similarities with the SMR-HB process in its initial stages.

The hydrogen generated is then directed toward ammonia production. Meanwhile, the captured carbon dioxide is separated from the syngas using techniques such as absorption, adsorption, or membrane separation. The purified carbon dioxide is transported to storage sites, typically via pipelines, which are favored for their ability to efficiently move the gas over long distances while benefiting from economies of scale. For shorter distances, specialized trucks can also be employed for transportation.

At the storage site, the carbon dioxide is injected into geological formations, including deep saline aquifers, depleted oil and gas reservoirs, or unmineable coal seams [17]. Alternatively, it can be utilized in tertiary oil recovery processes to enhance production rates [18].

In contrast, the LAC process differs significantly from the KBR process due to its unique configuration of process units. Unlike the KBR and SMR processes, which use both primary and secondary reactors, the LAC process employs only a primary reactor. The syngas mixture of hydrogen and carbon monoxide produced in this reactor undergoes an isothermal shift reaction, which generates additional hydrogen from carbon monoxide. The resulting syngas is then sent through the WGS process to

further increase hydrogen production.

Another distinguishing feature of the LAC process is the use of a dedicated cryogenic unit to generate nitrogen for the synthesis reaction, rather than sourcing it directly from the air. After the WGS reaction, carbon dioxide is separated from the syngas using absorption, adsorption, or membrane separation techniques. The separated carbon dioxide can then be transported for storage or utilization.

Following carbon dioxide removal, the hydrogen undergoes purification in a Pressure Swing Adsorption (PSA) unit to eliminate impurities. The purified hydrogen is subsequently directed to the Haber-Bosch process for ammonia synthesis, where nitrogen from the cryogenic unit is also utilized. Thus, the LAC process stands apart from the KBR process by integrating primary reforming, cryogenic nitrogen generation, isothermal shift reactions, carbon dioxide absorption, and PSA purification.

The GSR-NH₃ process, on the other hand, adopts yet another configuration for ammonia production. In this method, methane is reformed in a fluidized bed reactor, which replaces the primary and secondary reactors used in the SMR and KBR processes. The resulting syngas mixture of hydrogen and carbon monoxide is sent to a WGS reactor, where the reaction increases hydrogen production. The hydrogen is then purified in a PSA reactor before being fed into the ammonia synthesis loop [20].

The WGS reaction plays a key role in hydrogen production by facilitating the conversion of carbon monoxide and steam into carbon dioxide and hydrogen, as shown in the equation:



Here, *CO* stands for carbon monoxide, *H₂O* represents the steam produced from hot water, *CO₂* is the carbon dioxide, and *H₂* is hydrogen.

Following this reaction, carbon dioxide is separated from the gas stream. Once captured, it can be transported for storage or repurposed for various industrial applications.

3.2. Green Hydrogen and Ammonia Production (Electrolysis)

Combining water electrolysis with the Haber-Bosch process is an alternate method of producing ammonia (Lee et al., 2021). In this method, water serves as the primary feedstock. It is fed into an electrolyzer, where an electric current is applied to split the water molecules into hydrogen and oxygen.

The reaction can be expressed as:



Here, *H₂O* represents water, *H₂* indicates two molecules of hydrogen, and *O₂* stands for oxygen.

The electrolysis process initiates an oxidation reaction at the anode, where negatively charged ions (anions) are drawn to the positively charged electrode, releasing oxygen gas. Simultaneously, at the cathode, positively charged ions (cations) are attracted to the negatively charged electrode, resulting in the generation of hydrogen gas. This entire process requires an external electrical power source, which can be supplied by renewable energy technologies such as solar panels or wind turbines, depending on the project developer's preference.

Following electrolysis, the produced hydrogen gas must undergo purification to eliminate residual moisture, oxygen, and other impurities. This purification is typically carried out using PSA units, which ensure the hydrogen meets the required purity standards for subsequent use.

In parallel, nitrogen is extracted for use in downstream applications. This is achieved through cryogenic air separation units, which isolate and collect high-purity nitrogen from the air. Once purified hydrogen and nitrogen are available, they are combined in the Haber-Bosch process to synthesize ammonia.

Adjusting existing production facilities to manufacture blue and green ammonia involves significant modifications, which translate into increased capital and operational expenses for developers. The next section will explore the economic policies necessary to incentivize these investments and promote the reduction of carbon dioxide emissions within the ammonia production sector.

Economic Financing Measures to Mitigate Ammonia's GHG Emissions

Combining CCSU technologies with the SMR-HB process has the potential to significantly cut carbon dioxide emissions from ammonia production. However, the costs associated with implementing these changes can differ across countries and are influenced by several factors. These include the plant's capacity, the specific CCSU technologies adopted, the type of catalyst used, the extent to which excess heat is recovered and reused within the system, and the overall operational expenses of running the facility.

Retrofitting an existing ammonia plant with new infrastructure; such as a carbon dioxide absorption system, a cryogenic purification unit, or replacing traditional primary and secondary reactors with advanced alternatives like fluidized bed reactors; can lead to a substantial rise in capital expenditures. Even more so, transitioning to a completely reconfigured system, such as producing ammonia through electrolyzers powered by renewable energy, would further escalate these costs.

According to, the total capital investment required for integrating carbon capture into the SMR-HB process is estimated at approximately US\$831 million. This reflects the significant financial burden that such modifications impose on ammonia producers. As such, a long-term financing instrument would be required. Thus, green bonds emerge as an appropriate financing

tool as they can be used to mobilize sufficient capital funds and they can be structured with a long maturity to ease the burden for repayment.

The next subsection ventured into green bonds.

Green Bonds

A green bond is a fixed-income security designed to fund projects that deliver environmental benefits. While it shares key features with traditional bonds; such as a par value, coupon rate, and maturity date; its defining characteristic lies in the use of proceeds. Funds raised through green bonds are specifically allocated to environmentally beneficial projects [21]. In the ammonia industry, these could include integrating CCSU technologies with the Haber-Bosch process or financing the production of green ammonia via water electrolysis. Green bonds have several characteristics. They are as follows.

The first characteristic is the purpose and the use of proceeds. In fact, the purpose and use of proceeds is one of the distinguishing characteristics of green bonds from traditional (vanilla) bonds. The proceeds from green bonds are used for funding environmentally friendly projects [22].

The second characteristic is the certification and verification. To facilitate transparency and credibility, green bonds must adhere to guidelines set by the International Capital Market Association (ICMA), known as the Green Bond Principles (GBP). These principles require rigorous certification and verification processes, often conducted by independent third-party agencies. This validation assures investors that their capital is being directed toward genuine environmental projects [23].

The third characteristic is the coupon rate. The coupon rate of a green bond is influenced by market conditions, the issuer's creditworthiness, and the perceived risk of the bond. However, investors with an environmental focus may accept lower interest rates compared to traditional vanilla bonds, provided they are confident that the proceeds will be used for their intended purpose [24].

The fourth characteristic is the maturity. While the maturity of green bonds does not inherently differ from conventional vanilla bonds, issuers may negotiate longer repayment terms with project developers [25].

This flexibility can help align the bond's duration with the extended timelines typical of large-scale decarbonization projects.

The fifth characteristic is the report requirements. Green bonds typically come with stringent reporting obligations [26]. Issuers of green bonds for ammonia decarbonization projects are likely required to provide detailed disclosures on several aspects, including: i) how the bond proceeds are allocated and utilized; ii) the financial viability of the funded projects; iii) the volume of carbon dioxide emissions reduced; and iv) the overall environmental impact achieved.

Forecast of Ammonia Prices

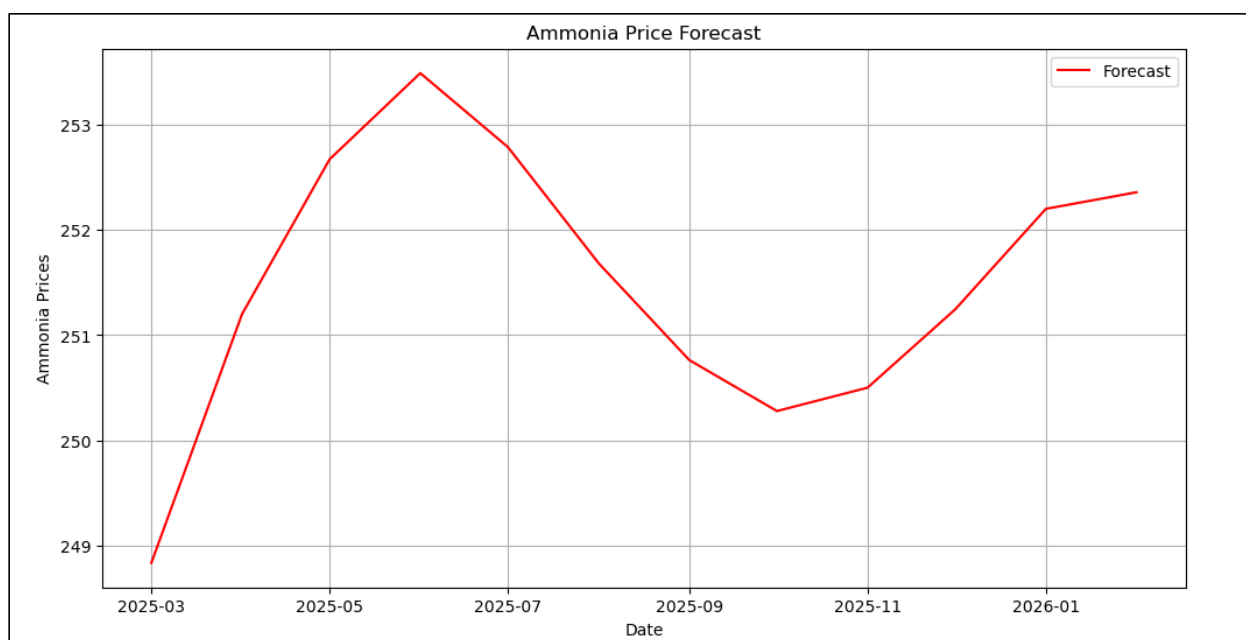


Figure 1: Forecast of Ammonia Prices (US\$/ton)

The forecasted ammonia prices from March 2025 to February 2026 indicate a moderate upward trend, with prices beginning at approximately US \$248.84 per ton in March 2025 and reaching around USD 252.36 per ton by February 2026. The forecast suggests a peak around mid-2025 (June), followed by a minor dip and then relative stabilization in the latter half of the forecast period. This stable to modestly increasing price trend has implications for the performance of a tokenized indexed green bond that is linked to the spot price of ammonia.

Such a bond, by design, provides a base coupon rate plus a premium that is positively correlated with ammonia prices. As a result, the gradual increase in prices over the forecast horizon implies that investors will likely benefit from rising coupon payments, particularly in the early months of the bond's lifecycle. This performance-linked structure creates an incentive for investors to support decarbonization efforts, as the proceeds of the bond are earmarked for financing green ammonia production. The higher the ammonia price, the greater the coupon and the corresponding financial benefit to the bond holders.

In traditional bond markets, the lot size or unit denomination typically refers to the face value of a single bond unit. The minimum tradeable lot is often US\$100,000, especially in over-the-counter (OTC) markets, making them inaccessible to small scale investors. However, tokenization allows the minimum bond unit (1 token) to be as low as a few dollars. For example, a US\$10 million bond could be split into 1 million tokens, making 1 token equal to US\$10. The lot size can be defined by the issuer of the bond and can be programed into the smart contract.

Discussion and Conclusion

The first research objective of this study was to examine the various methods available for reducing GHG emissions within the

ammonia industry. Decarbonization in this sector relies on the implementation of capital-intensive projects, with two primary pathways emerging. The first is the production of blue ammonia, which involves integrating CCSU technologies with the Haber-Bosch process. Several methodologies exist for producing blue ammonia, each utilizing different configurations of process units. Despite these variations, all approaches aim to reduce carbon dioxide emissions effectively.

Alternatively, decarbonization can be achieved through the production of green ammonia. This method involves using water electrolysis to produce hydrogen, which is then processed through the Haber-Bosch system to synthesize ammonia. While this approach also reduces carbon dioxide emissions, it comes with significant costs, often amounting to millions of dollars. The high capital requirements for both blue and green ammonia projects mean that project developers may take several years to recover their initial investments. Given this financial challenge, long-term financing mechanisms are essential. Green bonds, particularly tokenized indexed green bonds, emerge as a viable solution to bridge the funding gap.

The second research objective focused on considering green bonds as policy tools to foster an enabling environment for decarbonizing the ammonia industry. Both blue and green ammonia projects require strong financing mechanisms to support their implementation. Tokenized indexed green bonds, which link coupon payments to the spot price of ammonia, are proposed as an appropriate tool for this purpose.

A sub-objective of the study involved forecasting ammonia prices. The analysis suggests a stable to modestly increasing price trend, which has implications for the performance of tokenized indexed green bonds. These bonds offer a base coupon rate plus

a premium that rises with ammonia prices. Consequently, the projected gradual increase in ammonia prices implies that investors will likely benefit from higher coupon payments, especially during the bond's early lifecycle. This performance-linked structure incentivizes investment in decarbonization efforts, as proceeds are earmarked for financing green ammonia production. Higher ammonia prices translate to greater financial returns for bondholders, aligning investor interests with environmental goals.

In traditional bond markets, tradeable units often have high minimum denominations, making them inaccessible to small-scale investors. However, tokenization addresses this issue by allowing bonds to be divided into smaller units. For instance, a multimillion-dollar bond could be split into millions of tokens, with each token representing ownership of a fraction of the bond. The issuer can define the minimum lot size and program it into a smart contract, making green bonds more inclusive and accessible to a broader range of investors.

This study makes an empirical contribution by applying the LSTM model to forecast ammonia prices. Additionally, it provides a policy-oriented contribution by proposing the use of tokenized, indexed green bonds as a financing tool for ammonia decarbonization projects. While green and indexed bond markets currently exist, and tokenized bonds is an emerging tool. This study advocates for the combination of the strengths of these instruments by use of tokenized, indexed green bonds.

Such bonds offer several advantages: they can be fractionalized, enabling a wide range of investors, including small-scale participants, to invest in the bond. The coupon payments are indexed to the spot price of ammonia, which can attract potential investors seeking performance-linked returns. Furthermore, the proceeds from these bonds can be earmarked to fund decarbonization projects in the ammonia industry, supporting the transition to a green and low-carbon economy.

Appendix Data

The data on the spot price of ammonia is obtained at the monthly frequency from the Central Bank of Trinidad and Tobago (CBTT) database. The data covered the period January 1991 to February 2025, producing 410 observations.

Pretesting

Before the data is forecasted, some pretests are applied to determine if the data is linear or normally distributed. This is a necessary step since if the data is non-linear or not normally distributed, then models based on the linearity and normality assumptions would not be appropriate for the regression. The Jarque–Bera test for normality is applied. This test investigates normality through a joint null hypothesis of the skewness being equal to zero and the excess kurtosis being equal to zero.

The Bai-Perron tests of $L+1$ vs. L sequentially determined breaks is a test to determine the number of structural breaks in a time series by repeatedly testing if adding an additional break

improves the fit of the model.

Methodology: LSTM

Long Short-Term Memory (LSTM) networks are a specialized type of Recurrent Neural Network (RNN) designed to address the challenges of vanishing or exploding gradients that often arise in traditional RNNs during feedback loop operations [29–31].

In a standard RNN, the hidden state evolves as:

$$h_t = \tanh(W_h h_{t-1} + W_x x_t + b) \quad (\text{A.1})$$

However, because of the frequent nonlinear transformations, this formulation has the vanishing/exploding gradient problem.

To get around this, LSTMs define gates, which are parametric functions that control the flow of information. The sigmoid activation function $\sigma(z) = \frac{1}{1+e^{-z}}$

which is used by each gate. It converts inputs into $[0,1]$.

The forget gate regulates the amount of prior memories C_{t-1} is kept.

$$f_t = \sigma(W_f * [h_{t-1}, x_t] + b_f) \quad (\text{A.2})$$

where $\sigma(\cdot)$ is the sigmoid activation function, mapping values into $[0,1]$; W_f is the weight matrix mapping the forget gate; h_{t-1} is the 1 period lag of the hidden state (the output of the LSTM at time t); x_t is the input vector at time t ; b_f is the bias term for the forget gate.

The input gate controls the amount of fresh data that enters the cell.

$$i_t = \sigma(W_i * [h_{t-1}, x_t] + b_i) \quad (\text{A.3})$$

where $\sigma(\cdot)$ is the sigmoid activation function; W_i is the weight matrix mapping the input gate; h_{t-1} is the 1 period lag of the hidden state; b_i is the bias term for the input gate.

The new candidate information, or candidate memory state, is produced as follows:

$$\tilde{C}_t = \text{hanh}(W_c * [h_{t-1}, x_t] + b_c) \quad (\text{A.4})$$

where $\tilde{C}_t$ is the candidate memory state; $\text{hanh}(\cdot)$ is the hyperbolic tangent activation function; W_c is the weight matrix mapping the candidate gate; and b_c is the bias for the candidate gate.

Next, a weighted mixture of the new candidate and the old memory is used to update the cell state:

$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t \quad (\text{A.5})$$

where C_t is the cell state (memory) at time t ; $\odot$ is the dot operator for element-wise multiplication.

The memory section that contributes to the concealed state is determined by the output gate.

$$o_t = \sigma(W_o * [h_{t-1}, x_t] + b_o) \quad (\text{A.6})$$

where o_t is the output gate; W_o is the weight matrix for the output gate; and b_o is the bias for the output gate.

The hidden state at time t is specified as:

$$h_t = o_t \odot \tanh(C_t) \quad (\text{A.7})$$

where h_t is the hidden state; o_t is the output gate; $\odot$ is the dot operator for element-wise multiplication; $\tanh(\cdot)$ is the hyperbolic tangent activation function; C_t is the cell state (memory).

These formulas guarantee that the gradient $\frac{\partial C_t}{\partial C_{t-1}} = f_t$

can stay around 1 to avoid vanishing slopes when $f_t \approx 1$.

Selective forgetting is made possible via the gating mechanism (via f_t), upgrading (via i_t), as well as output control (via o_t), so solidity and flexibility are balanced.

LSTMs are appropriate for sequence modeling tasks like language modeling, time series forecasting, and speech recognition since the recurrence can be unrolled for several time steps.

Formally, a nonlinear dynamical system can be used to express the recurrence relation:

$$(h_t, C_t) = \Phi(h_{t-1}, C_{t-1}, x_t; \theta) \quad (\text{A.8})$$

where Φ is the LSTM update function parametrized by weights. $\theta = \{W_f, W_i, W_c, W_o\}$

Compared to the standard RNN, the error in the LSTM is stabilized

$$\frac{\partial L}{\partial C_{t-k}} = \prod_{j=1}^k f_{t-j+1} * \frac{\partial L}{\partial C_t} \quad (\text{A.9})$$

It maintains gradients over lengthy periods when $f_j \approx 1$

Therefore, LSTMs provide efficient learning across extended temporal horizons by combining additive memory updates with multiplicative gating functions.

The Python code for the LSTM model is available at

Pretesting Results

Jarque-Bera Test Statistic: 679.8371956448742

p-value: 2.3726226357482433e-148

The results suggest that rejection of the null hypothesis of normality. This suggests that the data does not follow a normal distribution

Table A1: Bai-Perron tests of L+1 vs. L Sequentially Determined Breaks

Sequential F-statistic determined breaks:			4
		Scaled	Critical
Break Test	F-statistic	F-statistic	Value**
0 vs. 1 *	224.6569	224.6569	8.58
1 vs. 2 *	44.82292	44.82292	10.13
2 vs. 3 *	51.99007	51.99007	11.14
3 vs. 4 *	26.47915	26.47915	11.83
4 vs. 5	0.935505	0.935505	12.25
* Significant at the 0.05 level.			
** Bai-Perron (Econometric Journal, 2003) critical values.			
Break dates:			
	Sequential	Repartition	
1	2007M12	2002M11	
2	2020M02	2008M01	
3	2015M01	2015M01	
4	2002M11	2020M02	

The results of the Bai-Perron tests of L+1 vs. L sequentially determined breaks suggests that there are 4 structural breaks. This was determined, as the null hypothesis of 0 breaks was rejected in favor of at least 1 break. The test was continued until the null hypothesis was 4 breaks and the alternate hypothesis was 5 breaks. The tests statistic was 0.935505 which was less than the critical value of 12.25, leading to the non-rejection of the null hypothesis of 4 structural breaks.

Diagnostics Results

As see in Figure A2, the Predictions with a 95% Confidence Interval and with error bands, provide a range of values within which the true value of the prediction is expected to lie with 95% confidence. This means that if the prediction process were repeated multiple times, 95% of the calculated confidence intervals would contain the true value. The results reveal that the majority of the time series falls within the confidence interval suggesting a good predictive accuracy of the model.

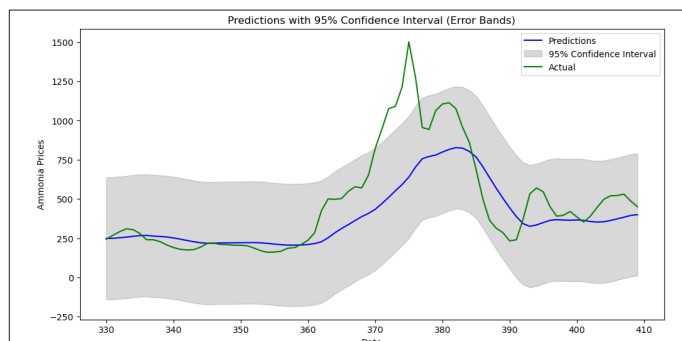


Figure A2: Predictions with 95% Confidence Interval

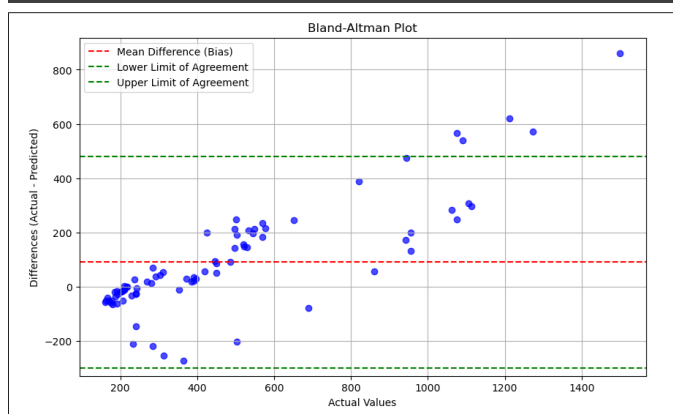


Figure A3: Bland-Altman Plot

Figure A3 shows the results of the Bland-Altman Plot. It evaluates the agreement between the ammonia price forecasts from the LSTM model and the actual observed prices, providing insights into the model's accuracy. The mean difference (bias) indicates whether the model systematically overestimates or underestimates ammonia prices; a value close to zero suggests minimal bias, while a non-zero value implies a consistent tendency to deviate in one direction. The upper and lower limits of agreement (± 1.96 standard deviations from the mean difference) define the range within which 95% of the prediction errors are expected to fall. The presence of 5 data points outside the 95% limits of agreement reveals outliers where the model's forecasts deviate significantly from the actual prices. However, this is understandable since commodity prices, including ammonia prices, respond to unexpected and changing macroeconomic factors. Models generally are not able to predict unexpected factors that can impact a commodity's price[32,33].

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