

Optimal Transition of Ammonia Supply Chain Networks via Stochastic Programming

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ABSTRACT

This paper considers the optimal incorporation of renewable ammonia production facilities into existing supply chain networks which import ammonia from conventional producers while accounting for uncertainty in this conventional ammonia price. We model the supply chain transition problem as a two-stage stochastic optimization problem which is formulated as a Mixed Integer Linear Programming problem. We apply the proposed approach to a case study on Minnesota's ammonia supply chain. We find that accounting for conventional price uncertainty leads to earlier incorporation of in-state renewable production sites in the supply chain network and a reduction in the quantity and cost of conventional ammonia imported over the supply chain transition horizon. These results show that local renewable ammonia production can act as a hedge against the volatility of the conventional ammonia market.

Keywords: Design and Sustainability, Stochastic Optimization, Capacity Expansion, Supply Chain Optimization, Green Ammonia

INTRODUCTION

Ammonia is one of the most important industrial chemicals and serves as the backbone of modern agriculture in its use either directly or as a precursor to other nitrogen fertilizers. The standard production of ammonia is based on the Haber-Bosch process, which uses fossil fuels as the feedstock hydrogen source and operates at high pressure and temperature [1]. These facilities generally have capacities greater than 1,000,000 metric tons per year (mt/y) to take advantage of economies of scale [2]. This production paradigm leads to high transportation costs and carbon emissions in the operation of the supply chain because ammonia is transported through national and even global networks of ships, pipelines, rail, and trucks from a few production sites to the final customers [3].

The transition to a more sustainable supply chain network can be achieved by reducing the carbon emissions related to the manufacturing and distribution of ammonia. Renewable or green ammonia production recently has been the subject of extensive research and development as an alternative to the standard ammonia manufacturing paradigm [4]. In this approach, renewable

resources such as wind and solar are used to produce hydrogen via electrolysis and nitrogen via air separation, reducing the carbon intensity of producing ammonia. The Midwest region of the United States uses the most nitrogen fertilizer in the country while also being home to rich wind resources [5]. This gives rise to an opportunity to produce renewable ammonia closer to where it is used, thus reducing the cost and carbon intensity of ammonia distribution [6]. Producing ammonia using renewable energy also offers the potential for ammonia production cost stability. The feedstock renewable energy can have a close-to-constant price in this production setting, whether this energy is sourced through multi-year power purchase agreements (PPA) or the ammonia producer owns and operates the necessary renewable generation. In contrast, ammonia is currently traded on a global market and its price is subject to variability due to a number of factors including natural gas prices, food prices, and global conflict (see Figure 1). Given the transformative potential of renewable ammonia, achieving economical deployment through optimal design of manufacturing facilities and the supply chain network is of critical importance. In this work, we focus on the latter.

The transition of existing ammonia supply chain

networks to incorporate renewable production will likely occur over multiple years and will be affected by multiple sources of uncertainty. Identifying optimal investment decisions over a fixed planning horizon is a widely studied problem in process systems engineering and operations research and is formally known as the capacity expansion problem [7]. However, the application of the capacity expansion formalism to the transition of ammonia supply chain networks is rather limited. Recently, we have proposed a multiperiod deterministic capacity expansion model that considers the optimal transition of ammonia supply chain networks [8]. The model optimizes the investment decisions regarding the installation year and capacity, such that the overall net present cost is minimized while ammonia fertilizer demand is satisfied.

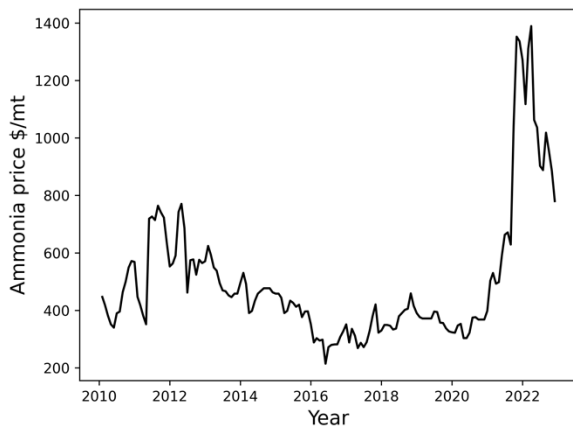


Figure 1. U.S. Gulf Coast ammonia price from 2010 to 2022 [9].

In this work, we consider the effect of uncertainty on the optimal transition of existing ammonia supply chain networks. The primary sources of uncertainty in an ammonia supply chain are the ammonia demand and the market price of ammonia. Although the demand for ammonia can be predicted from total fertilizer demand estimates, the ammonia price is more volatile. Accounting for the significant price variability and uncertainty is essential for the optimal expansion of existing supply chain networks.

We propose a two-stage stochastic programming approach where the uncertainty in price is accounted for in the form of scenarios [10,11]. Such a conceptual approach has been previously employed in supply chain optimization models in a number of different industries, for example, waste-to-bioethanol [12], biodiesel production from wastewater treatment byproducts [13], and coal-to-liquids [14]. In our model, the installation decisions (the location, capacity, and construction year for new renewable ammonia manufacturing facilities) are the first stage decisions, and the distribution of ammonia from the installed renewable sites and the conventional producers

to the customers for the different ammonia prices (scenarios) are the second stage decisions. We consider a case study on Minnesota's ammonia supply chain network. The results show that accounting for uncertainty in the price of ammonia, especially high prices, requires investments earlier in the planning horizon, compared to assuming a nominal price. Furthermore, we simulate the supply chain obtained from the deterministic and stochastic models, and we find that for high ammonia prices, the design obtained via stochastic programming results in lower net present costs. These results highlight the ability of locally-produced renewable ammonia to act as a hedge against high prices on the conventional ammonia market. The rest of the paper is organized as follows: First, we present the two-stage stochastic optimization model, then we present the case study and, finally, the numerical results.

TWO-STAGE STOCHASTIC OPTIMIZATION MODEL

We consider an existing supply chain network that delivers ammonia to a set of counties $\mathcal{C} = \{1, \dots, C\}$ via distribution centers $\mathcal{D} = \{1, \dots, D\}$. In the original network, the demand δ_c at each county is satisfied by purchasing ammonia from conventional producers $\mathcal{P} = \{1, \dots, P\}$ with price α_p . Given a set of candidate locations for renewable ammonia production facilities $\mathcal{R} = \{1, \dots, R\}$, the goal is to find the optimal investment decisions over a planning horizon $\mathcal{K}$, such that the total net present cost of the supply chain is minimized, demands are met for each period of the planning horizon, and at the end of the horizon the entire demand is satisfied using renewable ammonia. We assume that the capacity investment decisions are made annually and the planning horizon $\mathcal{K}$ is discretized into K time periods. We define variable x_{rk} as the capacity installed at candidate renewable site r at time period k , and binary variable z_{rk} which is equal to one if an investment is made at candidate site r at time period k and zero otherwise. We assume that the only uncertain parameter is the price of ammonia imported from conventional producers. We model the renewable ammonia production investment decisions, specifically the time period when an investment is made z_{rk} and the production capacity x_{rk} at a given candidate location r , as first-stage decisions. The amount of ammonia sent to each county through a combination of purchases from conventional producers routed through distribution centers and from new renewable production facilities are the second stage decisions. We follow a scenario-based formulation and define the set $\mathcal{S} = \{1, \dots, S\}$ which represents the scenarios of the price of ammonia, where each scenario has probability p_s , and the price of ammonia for producer p and scenario s is α_{ps} .

Given this problem setting, first, we define

constraints related to the maximum and minimum capacity that can be installed in each location and time period by the following constraints

$$x_{rk} \leq \bar{x}^U z_{rk} \quad \forall r \in \mathcal{R}, k \in \mathcal{K} \quad (1)$$

$$x_{rk} \geq \bar{x}^L z_{rk} \quad \forall r \in \mathcal{R}, k \in \mathcal{K}, \quad (2)$$

where $\bar{x}^U, \bar{x}^L$ are the upper and lower bounds on the size of renewable sites. Each renewable candidate site has a certain wind capacity Ω_r , electrolysis capacity Ω_k , and a construction period of two years, which constrain the maximum capacity that can be installed and the time that the capacity is available as follows

$$\sum_{k'=1}^k x_{rk'} \omega_{rk'} \leq \Omega_r \quad \forall r \in \mathcal{R}, k \in \mathcal{K} \quad (3)$$

$$\sum_{r \in \mathcal{R}} x_{rk} \xi_{rk} \leq \Xi_k \quad \forall k \in \mathcal{K}. \quad (4)$$

We define variable y_{pdks} as the amount of ammonia purchased from conventional producer p and shipped to distribution center d at time period k and scenario s . We also define variable y_{dcks} as the amount of ammonia shipped from distribution center d to county c at time period k and scenario s , and the amount of ammonia shipped from the renewable site r to county c at time period k and scenario s is y_{rcks} . The demand satisfaction constraints are

$$\sum_{r \in \mathcal{R}} y_{rcks} + \sum_{d \in \mathcal{D}} y_{dcks} \geq \delta_{ck} \quad \forall s \in \mathcal{S}, c \in \mathcal{C}, k \in \mathcal{K} \quad (5)$$

$$\sum_{p \in \mathcal{P}} y_{pdks} \geq \sum_{c \in \mathcal{C}} y_{dcks} \quad \forall s \in \mathcal{S}, d \in \mathcal{D}, k \in \mathcal{K} \quad (6)$$

$$\sum_{d \in \mathcal{D}} y_{pdks} \leq \Lambda_p \quad \forall s \in \mathcal{S}, p \in \mathcal{P}, k \in \mathcal{K} \quad (7)$$

$$\sum_{c \in \mathcal{C}} y_{rcks} \leq \sum_{k'=1}^{k-2} x_{rk'} \quad \forall s \in \mathcal{S}, r \in \mathcal{R}, k \in \mathcal{K} \quad (8)$$

$$\sum_{p \in \mathcal{P}} \sum_{d \in \mathcal{D}} y_{pdks} = 0 \quad \forall s \in \mathcal{S}. \quad (9)$$

The objective function is the net present cost of the supply chain transition over the planning horizon. It can be partitioned into two terms. The first term, Z_k , is the sum of the capital CAP_k and operating costs OP_k which depends only on the first-stage decisions, and are computed as follows

$$CAP_k = \frac{1}{\theta} \sum_{r \in \mathcal{R}} \sum_{k'=1}^k x_{rk'} \sigma_{rk'} + z_{rk'} \gamma_{rk'} \quad (10)$$

$$OP_k = \sum_{r \in \mathcal{R}} \sum_{k'=1}^k x_{rk'} \zeta_{rk'}. \quad (11)$$

The capital cost of a renewable production facility is modeled as a piece-wise affine function of the installed capacity, with slope σ_{rk} and intercept γ_{rk} , to capture the effect of economies of scale. These parameters vary with both renewable site r and time period k to capture the effects of varying renewable potential and expected technology cost reductions respectively. The capital cost is annualized using scaled plant lifetime θ which is equal to 10.23 y^{-1} . The operating cost is assumed to scale linearly with the installed capacity with proportionality constant ζ_{rk} . This parameter is assumed to remain constant after installation and also varies with renewable site and

period to capture the effects described above.

The second term in the objective, $\bar{Z}_{ks}$, is the sum of the distribution of renewable ammonia DR_{ks} , transportation of ammonia from the conventional producers to the distribution centers TC_{ks} , and distribution of conventional ammonia DC_{ks} . The individual costs are equal to

$$DP_{ks} = \sum_{r \in \mathcal{R}} \sum_{c \in \mathcal{C}} y_{rcks} \tau_{rc} \quad \forall k \in \mathcal{K}, s \in \mathcal{S} \quad (12)$$

$$PC_{ks} = \sum_{p \in \mathcal{P}} \sum_{d \in \mathcal{D}} y_{pdks} \alpha_{ps} \quad \forall k \in \mathcal{K}, s \in \mathcal{S} \quad (13)$$

$$TC_{ks} = \sum_{p \in \mathcal{P}} \sum_{d \in \mathcal{D}} y_{pdks} \tau_{pd} \quad \forall k \in \mathcal{K}, s \in \mathcal{S} \quad (14)$$

$$DC_{ks} = \sum_{d \in \mathcal{D}} \sum_{c \in \mathcal{C}} y_{dcks} \tau_{dc} \quad \forall k \in \mathcal{K}, s \in \mathcal{S} \quad (15)$$

$$Z_k = CAP_k + OP_k \quad \forall k \in \mathcal{K} \quad (16)$$

$$\bar{Z}_{ks} = DC_{ks} + PC_{ks} + TC_{ks} + DP_{ks} \quad \forall k \in \mathcal{K}, s \in \mathcal{S}. \quad (17)$$

The two-stage optimization problem is

$$\begin{aligned} \min & \sum_{k \in \mathcal{K}} \phi_k Z_k + \sum_{s \in \mathcal{S}} \rho_s (\sum_{k \in \mathcal{K}} \phi_k \bar{Z}_{ks}) \\ \text{s. t.} & \text{Eq. 1} - 9 \end{aligned} \quad (18)$$

$$x_{rk} \geq 0, z_{rk} \in \{0,1\}$$

$$y_{rcks} \geq 0, y_{dcks} \geq 0, y_{pdks} \geq 0$$

The parameter ϕ_k is the discounted value of cost contributions in time period k .

CASE STUDY

We herein provide a concise description of the case study on Minnesota's ammonia supply chain. For a more detailed case study description, please refer to our previous work [8]. We consider a supply chain planning horizon from 2024 to 2032. We consider an 8.5% discount rate as it pertains to cost flows beyond 2024. Minnesota has 82 counties in which ammonia demand must be met for each period of the supply chain transition optimization. In 2024, the total ammonia demand assumed to be 795,000 mt/y and this is assumed to increase by 0.5% per year. This ammonia can be purchased from 10 conventional producers which are located outside of Minnesota. The average conventional ammonia price from 2010 to 2022 was \$500/mt. Ammonia purchased from these producers is routed through one of three distribution centers in Minnesota. Conventional producers located further from Minnesota have higher associated costs to transport ammonia to a given distribution center. Producer-to-distribution transportation costs range from \$59/mt to \$141/mt, while distribution center-to-county transportation costs range from \$1/mt to \$36/mt.

We consider 26 candidate locations for new in-state renewable ammonia production. Capital costs of a given facility are incurred two years before renewable production begins to represent a two year construction period. The operating cost includes renewable power purchases from PPAs with wind generators assumed to be co-

located with the renewable ammonia production facility. The operating cost also includes revenue from hydrogen production tax credits (PTCs) contained in the U.S. federal government Inflation Reduction Act [15]. These credits provide \$3/kg of hydrogen produced for the first 10 years of facility operation. Renewable ammonia is assumed to be transported from new production facilities directly to counties. These transportation costs range from \$1/mt to \$47/mt. The capacity of each new renewable ammonia facility is constrained to a maximum associated wind generation capacity of 250 MW (Eq. 3). The total installed capacity of renewable ammonia production across all facilities in a given year is constrained by electrolysis availability, which increases from 250 MW in 2024 to 850 MW in 2032 (Eq. 4). The optimization model is implemented in Pyomo [16] and is solved using Gurobi 10.0.2.0 [17] on an Apple MacBook Pro M1 with 8 physical cores and 16 GB of RAM.

NUMERICAL RESULTS

Deterministic case

First, we solve a deterministic model using a \$500/mt historical average conventional ammonia price, i.e., using the two-stage model with one scenario with probability one and price \$500/mt. The optimization problem has 22,194 (234 binary and 21960 continuous) variables, 1,803 constraints and is solved in 6.7 seconds. The total net present cost is \$3,002 million (MM) and renewable ammonia production is installed at eight new sites, as presented in Table 1. Three renewable ammonia facilities are installed in 2027, meaning that in-state production does not begin until 2029 and all ammonia is purchased from the conventional market for the first five years of the planning horizon (see Figure 3).

Table 1: Installation year, location, and capacity for new renewable ammonia production in the deterministic case. Annual average wind capacity factors for each selected candidate location are provided in parentheses to describe wind potential.

Year	Location	Capacity (1,000 mt/y)
2027	Lake Wilson (52%)	121.4
2027	Chandler (52%)	121.4
2027	Worthington (52%)	55.2
2028	Luverne (52%)	121.2
2028	Wilmont (52%)	110.4
2028	Worthington (52%)	66.0
2030	Blue Earth (47%)	116.1
2030	Winnebago (47%)	114.8

Three additional facilities are installed in 2028. These first six facilities are all located in Southwest

Minnesota, which has the highest wind capacity factors at 52%. In both 2027 and 2028, 575 MW of electrolysis is procured, the maximum allowable amount in each year. This is the reason that two smaller facilities are installed in Worthington in consecutive years. The final facilities are installed in 2030 to ensure that all ammonia is obtained via renewable production by 2032. These are both installed in Southeast Minnesota, which also has a high wind capacity factor at 47%. With the exception of the two smaller facilities in Worthington, all others use at least 225 MW of co-located wind generation in an attempt to achieve economies of scale.

Stochastic case

We use the data presented in Figure 1 and generate the histogram presented in Figure 2 using ten bins, and obtain the price at the edge of each bin and the number of data points in each bin. Given these data, we generate the scenarios where the price of ammonia in scenario s is set equal to the edge price in the bin s and the probability p_s is the number of data points in the bin s divided by the total number of data points.

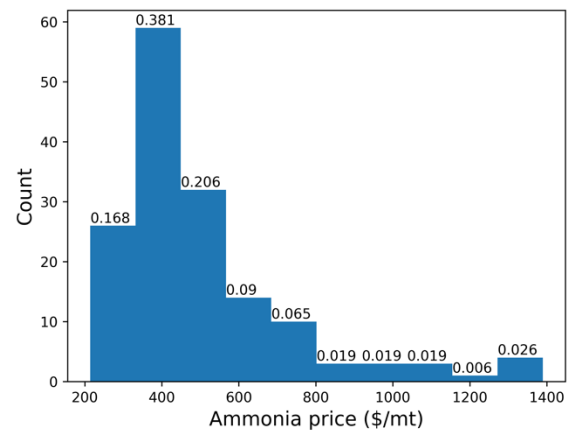


Figure 2. Histogram of U.S. Gulf Coast ammonia prices from 2010 to 2022. The width of each histogram bin is \$117.5/mt. In the stochastic optimization model, the probability of the conventional ammonia price being within each bin is listed above that bin.

The optimization problem has 217,566 (234 binary and 217332 continuous) variables, 11,927 constraints, and the solution time is 78 seconds. The total net present cost is \$3,230MM and the renewable sites installed are presented in Table 2. As with the optimal solution of the deterministic model, eight new renewable production facilities are installed. However, these installations occur earlier in the optimal stochastic supply chain transition.

One new facility each is installed in 2024 and 2025, which allows some market penetration of renewable ammonia by 2026 (see Figure 3). Both of these facilities are

installed in locations with the highest wind potential and use the maximum allowable 250 MW of co-located wind generation capacity. In 2027, three additional facilities are added and these cumulatively use 575 MW of electrolysis, the upper bound for that year. The facilities in both Luverne and Worthington use 250 MW of wind generation. We point out that these facilities have slightly higher production capacity than those in Lake Wilson (2024) and Chandler (2025) due to the more efficient electrolysis expected to be available in future years. The third 2027 facility is located in Southeast Minnesota despite its lower wind potential, unlike in the deterministic supply chain. This enables another facility which uses 250 MW wind to be installed in Wilmont in 2028; all five facilities with the highest wind potential (52% capacity factor) use this maximum amount of wind capacity to achieve economies of scale. Another facility is installed in Southeast Minnesota in 2028, also at the 2050 MW scale. Finally, a smaller facility is installed in Southeast Minnesota in 2030 to ensure a fully renewable supply chain by 2032.

Table 2: Installation year, location, and capacity for new renewable ammonia production in the two-stage stochastic case. Annual average wind capacity factors for each selected candidate location are provided in parentheses to describe wind potential.

Year	Location	Capacity (1,000 mt/y)
2024	Lake Wilson (52%)	117.7
2025	Chandler (52%)	117.7
2027	Luverne (52%)	121.14
2027	Worthington (52%)	121.14
2027	Winnebago (47%)	50.71
2028	Wilmont (52%)	121.24
2028	Blue Earth (47%)	111.11
2030	Fairmont (47%)	65.34

Comparison between deterministic and stochastic cases

The optimal transition in the stochastic case results in less conventional ammonia purchases and more in-state renewable production over the planning horizon compared to the deterministic transition. This difference leads to a reduction in the total amount of ammonia purchased leading to lower cumulative purchase, transportation, and distribution costs for conventional ammonia over the planning horizon (see Figure 4). Conversely, the capital cost for renewable ammonia production is higher in the stochastic transition even though the same total capacity of renewable production is installed in both cases. This is due to earlier installation using more expensive constituent technologies in the stochastic case.

This also contributes to higher renewable ammonia operating costs over the planning horizon, though these are also higher simply because more renewable ammonia is being produced. Overall, the net present cost of the supply chain transition is 7.6% (228 MM\$) higher in the stochastic case than the deterministic case.

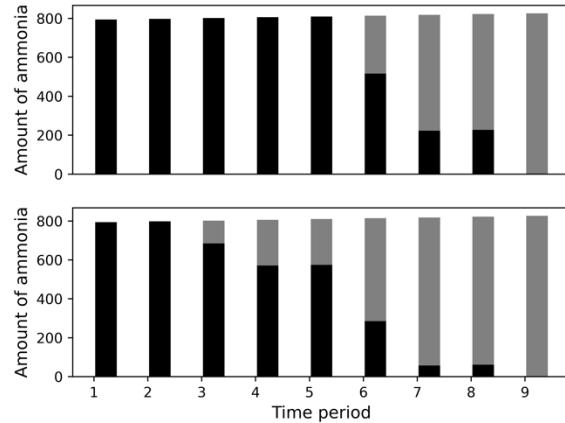


Figure 3. Amount of ammonia (mt) in each time period from conventional purchases (black bar) and in-state renewable ammonia production (gray bar) for the deterministic (top figure) and stochastic (bottom figure) cases.

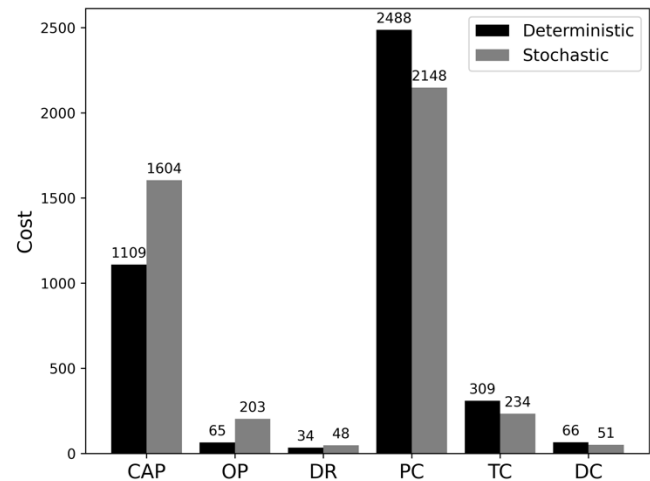


Figure 4. Cost contributions to optimal net present cost for the deterministic and stochastic cases. The cost acronyms are defined as follows: CAP - Renewable capital, OP - Renewable operating, DR - Renewable distribution, PC - Conventional purchase, TC - Conventional transportation to Minnesota, DC - Conventional distribution.

We compare the supply chain configurations obtained via the deterministic and stochastic transition optimizations for different conventional ammonia prices to

elucidate the benefit of the stochastic approach. Specifically, we discretize the ammonia price uniformly in 100 points between \$214/mt and \$1389/mt, and for each price, we fix the investment decisions (timing of investments, i.e., binary variables and installed capacity) and compute the net present cost of supply chain transition (see Figure 5). We observe that for high prices of conventional ammonia (above \$700/mt), the net present cost of the supply chain obtained via stochastic programming is meaningfully lower than the cost of the deterministic design, whereas if the price is low (below \$400/mt) the design obtained by the deterministic model has a meaningfully lower net present cost. This difference can be attributed to the different investment strategies for the stochastic and deterministic cases (i.e., more ammonia is manufactured in-state for the stochastic case) as discussed in the previous paragraph.

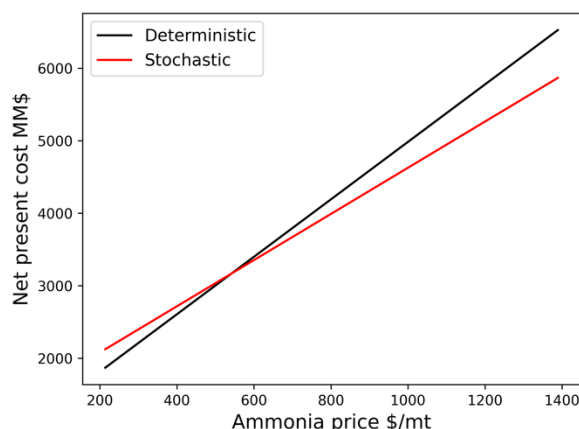


Figure 5. Levelized cost for the deterministic and stochastic design as a function of ammonia price.

CONCLUSIONS

In this work, we focused on quantifying the effect of uncertainty in conventional ammonia prices on Minnesota's transition from importing fossil-derived ammonia from out-of-state conventional producers to in-state renewable ammonia production. We used a two-stage stochastic programming approach to determine the optimal investment profile for in-state renewable ammonia production over a fixed planning horizon such that the demand of ammonia is satisfied while the net present cost is minimized. The results show that when accounting for uncertainty in the conventional ammonia price, investments are made earlier in the planning horizon compared to a deterministic supply chain transition model. This leads to a reduction in the amount of ammonia purchased from conventional producers. This can bring significant cost savings for higher-than-average ammonia prices. Overall, the stable production cost afforded by in-state

renewable ammonia production can act as a hedge against conventional ammonia price uncertainty and the possibility of very high prices on the conventional ammonia market.

This work used a two-stage approach to account for conventional price uncertainty, but in practice these prices could evolve different multi-year trajectories. Future work will therefore develop multi-stage stochastic programming models for the supply chain transition problem. Furthermore, technology cost reductions are also subject to uncertainty, especially further into a given planning horizon. For example, electrolysis costs are expected to decrease, but the magnitude of this reduction is not well-established at present. Thus, these types of uncertainties will also be incorporated into future supply chain transition models.

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