A Framework for Ammonia Supply Chain Optimization Incorporating Conventional and Renewable Generation

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Ammonia is an essential nutrient for global food production brought to farmers by a well-established supply chain. This article introduces a supply chain optimization framework which incorporates new renewable ammonia plants into the conventional ammonia supply chain. Both economic and environmental objectives are considered. The framework is then applied to two separate case studies analyzing the supply chains of Minnesota and Iowa, respectively. The base case results present an expected trade-off between cost, which favors purchasing ammonia from conventional plants, and emissions, which favor building distributed renewable ammonia plants. Further analysis of this trade-off shows that a carbon tax above $25/t will reduce emissions in the optimal supply chain through building large renewable plants. The importance of scale is emphasized through a Monte Carlo sensitivity analysis, as the largest scale renewable plants are selected most often in the optimal supply chain. © 2017 American Institute of Chemical Engineers *AIChE J*, 63: 4390–4402, 2017
Keywords: supply chain optimization, distributed ammonia production, wind power, green fertilizer

Introduction

Ammonia is one of the most essential chemicals existing today. Without it, there would be no way to ensure the nitrogen levels required to feed the growing human population. Anhydrous ammonia, a chemical which is 82% nitrogen, is often directly injected into the ground through a stake for use as fertilizer. Ammonia also has many other uses, for example as a precursor to nitrogenous commodity chemicals, as a chemical-based storage of energy,[1] as a way to store hydrogen as a liquid at reasonable temperatures and pressures,[2] and as a liquid fuel.[3] Clearly, demand for ammonia will only continue to grow in the future.[4]

The Haber-Bosch process revolutionized the ammonia industry on its discovery in the early 20th century. This process, however, requires hydrogen as an input. At present, this hydrogen is typically obtained from fossil fuels, using processes such as steam reforming of methane or coal gasification.[5] This presents two key sustainability issues: first, ammonia production presents an ever-present and increasing demand on a finite fossil fuel supply, and second, ammonia production contributes to global greenhouse gas emissions, which are believed to be an important factor underlying anthropogenic climate change. Thus, without the introduction of new processes, ammonia cannot be produced at the levels required to supply the growing human population in a sustainable manner.

Motivated by these concerns, a first of its kind pilot scale ammonia plant was recently built at the West Central Research and Outreach Center at the University of Minnesota. This plant produces the hydrogen required for ammonia through wind-powered electrolysis of water. The technology, with a flowsheet depicted in Figure 1, has been proven at the pilot scale.[6] In general, such wind-powered plants will likely be built at a smaller scale than their conventional counterparts which exist at scales as large as 2 million tons per year.[7] Although existing ammonia production is highly centralized, demand for nitrogen fertilizer is distributed all across the country, as shown in Figure 2.[8] This figure shows the acreage of farms growing corn, one of the highest ammonia demanding crops. Other critical crops requiring high amounts of ammonia as a source of nitrogen include wheat, barley, oats, and cotton. As such, it seemingly would make more sense to produce ammonia at a smaller scale and in a more distributed fashion to better match supply and demand.

In theory, any renewable energy source could be used to power this new renewable ammonia production process. However, Figure 3 can shed some light on why wind is the ideal

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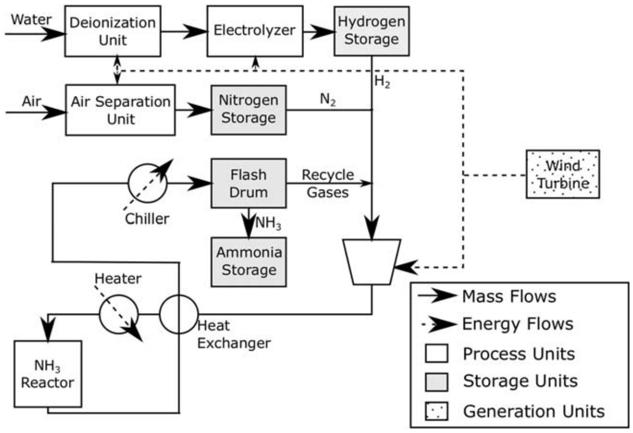

Figure 1. Process flowsheet for novel renewable ammonia system built in Morris, MN.

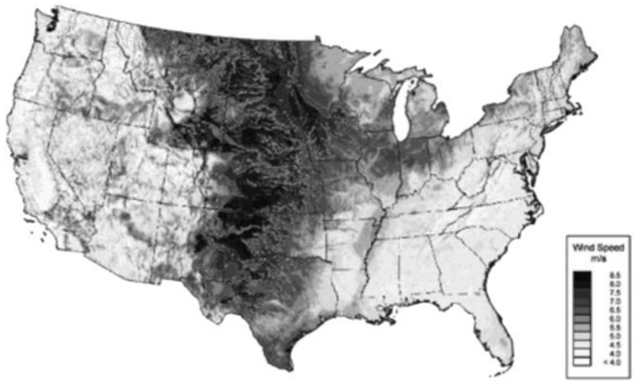

Figure 3. Wind resources in the United States.[9]

renewable source to choose.[9] In this figure, it is apparent that there is significant overlap between the areas with high wind potential and the areas with high ammonia demand in the United States. This overlap also occurs in other parts of the world, such as in Europe where many high potential wind areas overlap with high wheat producing locations. In addition, many of the areas with high wind potential are located in rural locales with low population density. As such, this energy is often referred to as "stranded" energy: energy located too far away from major population centers to be useful without incurring substantial transmission costs and losses. Distributed renewable ammonia production provides a use for this stranded energy, as it can be used directly onsite to produce ammonia, a product that is needed in these rural areas containing a high density of crops requiring anhydrous ammonia or other nitrogen fertilizer.

This article addresses two key questions concerning new renewable ammonia plants: Can such a renewable plant be economically competitive with existing conventional plants, and if so, at what scale are the plants competitive? To this end, the remainder of this article proposes a general framework for analyzing both conventional and renewable plants within the ammonia supply chain, and is structured as follows. First, some background is presented that reviews existing research on sustainable supply chains and summaries the current state of the ammonia supply chain. Next, the general mathematical optimization framework is introduced. We then present some preliminary data that will be used for the analysis of two case studies, which look at the ammonia supply chains of the states of Minnesota and Iowa, respectively. The results of these case studies are discussed in the following section. Finally, some concluding remarks and avenues for future work are presented.

Background

Supply chains consist of networks of material and information flows between different facility nodes.[10] The nodes often include suppliers, manufacturers, storage and distribution centers, and consumers, while the flows can occur through many different means of transportation, including trucks, barges, ships, planes, trains, and pipelines. Supply chain optimization, then, involves determining the best configuration of nodes and flows that will minimize a certain objective. There are many possible objectives that one could consider, but in the context of sustainable supply chains, typically a combination of

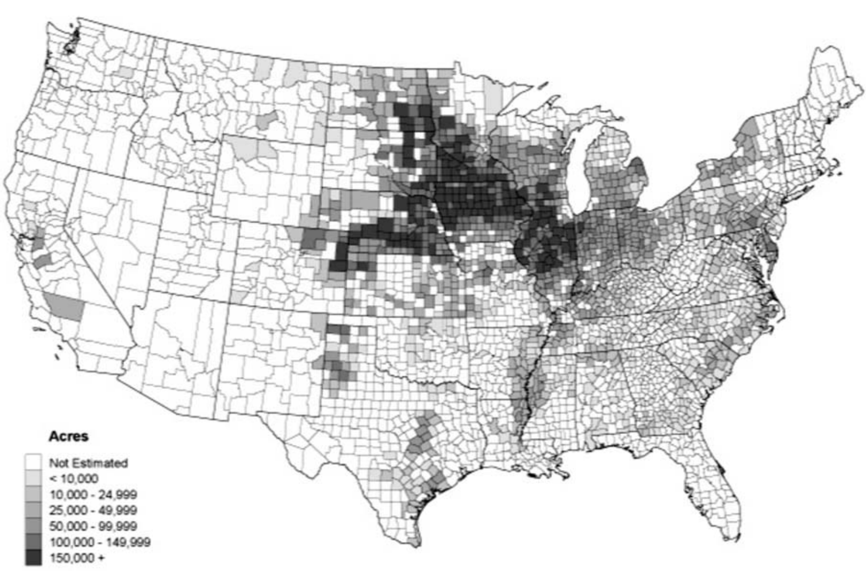

Figure 2. Amount of farmland used for corn production by county in the United States.[8]

economic, environmental, and social metrics, the so called "three pillars" of sustainability, are used.[11,12]

Supply chain optimization is of critical importance to industry and is particularly useful for new or expanding industries to understand, for example, how and where additional capacity integrates with established production. In the following paragraphs, we briefly review the use of supply chain optimization applied to several emerging renewable chemical industries. The most prevalent of these renewable chemical supply chains involve biofuels and biochemicals. The optimal design of biofuel supply chain networks considering uncertainties in various key parameters, such as local demand, market prices, and process yields, has been analyzed using a Monte Carlo approach to global sensitivity analysis.[13] Other previous work developed a generic framework for a bioethanol supply chain and applied this over a nine-state region in the upper midwest.[14] This work was extended to allow for selection between multiple biomass processing technologies as well as take into account existing corn biofuel plants in the analysis.[15] The implementation of distributed biofuel production has been examined via a novel small scale biodiesel production facility to satisfy local fuel demands in the greater London region.[16] Additional previous research has incorporated a multiobjective optimization of cellulosic biofuel supply chains, using a life cycle analysis that simultaneously considered economic, environmental, and social objectives.[17] This work was extended to analyze bioelectricity, instead of biofuel, using a similar multiobjective optimization with life cycle analysis approach.[18] A biofuel supply chain which incorporates existing petroleum infrastructure has also been previously studied, showing that incorporating existing petroleum production facilities and pipelines into the biofuel supply chain can result in a reduction of cost.[19]

Biofuels are not the only renewable chemical considered in supply chain optimization. Hydrogen supply chains considering both environmental and economic objectives have been investigated, which assume vehicle end use and different production, storage, and transportation technologies.[20] The sugar supply chain has also been considered in addition to bioethanol, as both are potential products of sugarcane.[21] A large scale carbon dioxide supply chain has been proposed to analyze carbon capture, storage, and sequestration and identify how best to reduce carbon emissions and utilize carbon dioxide for profits.[22] Ammonia supply chains, which we consider in this work, have received little attention, in large part because conventional ammonia production is a well-established technology. One study considered ammonia as a potential future energy carrier by taking into account the entire ammonia supply chain; however, this study focused on technoeconomic analysis rather than supply chain optimization.[23] An additional study considered ammonia as part of a supply chain optimization of a large-scale petrochemical complex, most of which is used as a precursor to urea production.[24]

In this work, we seek to develop a supply chain optimization model which analyzes an ammonia supply chain considering both existing conventional production and new production with renewably generated hydrogen ("renewable production") at candidate locations with existing wind capacity. In this sense, supply chain optimization is used here as a tool to provide a complete comparison of the economic and environmental costs of conventional vs. renewable ammonia production. The traditional ammonia supply chain consists of centralized conventional plants where ammonia is produced at large quantities, transported, typically by rail or pipeline, to local distribution centers, and then further transported by truck to local consumers.[25] This work considers the possibility of introducing local renewable ammonia plants into the traditional supply chain. Because these plants are being built locally, they can bypass the distribution centers and ship directly to the consumer, using either onsite storage or assuming the end user has sufficient storage. The remainder of this article develops and uses an optimization formulation to compare renewable and conventional ammonia production within the supply chain.

Problem Formulation

In this section, an optimization framework is developed that considers the existing ammonia supply chain and decides if and where to build renewable plants among candidate location sites, as well as how to transport ammonia through the supply chain. The formulation uses steady-state mass balances throughout the supply chain; in practice, this would be accomplished through adequate storage at production, distribution, and end use nodes. Ammonia can be purchased from existing conventional plants and then transported to one of the ammonia distribution centers. The total ammonia purchased from a conventional site may not exceed its maximum allowable value ξ_p

$$\sum_{d=1}^{D} y_{p,d} \leq \xi_p \quad \forall p \tag{1}$$

where $y_{p,d}$ is ammonia shipped from a conventional plant p to a distribution center d. From the distribution centers, ammonia is then further transported to local demand sites. At each distribution site, there is a mass balance for ammonia: distribution centers cannot ship out more ammonia than they receive from conventional plants

$$\sum_{p=1}^{P} y_{p,d} - \sum_{m=1}^{M} y_{d,m} \geq 0 \quad \forall d \tag{2}$$

where $y_{d,m}$ is the amount of ammonia shipped from a distribution center d to a final demand site m. Local ammonia demands can also be met by building a new renewable plant. If this occurs, the plant capacity built (x_r) may not exceed its maximum allowable value ξ_r

$$x_r \leq \xi_r \quad \forall r \tag{3}$$

As the renewable plant candidate sites are distributed and local, there is no need to transport this renewable ammonia to a distribution center; instead, it may be transported directly to the demand sites. Again, an ammonia mass balance must hold at each renewable plant, as the plant cannot ship out more ammonia than it produces

$$x_r - \sum_{m=1}^{M} y_{r,m} \geq 0 \quad \forall r \tag{4}$$

where $y_{r,m}$ is the amount of ammonia shipped from a renewable site r to a final demand site m. Regardless of whether renewably or conventionally produced ammonia is used to satisfy local demand, this demand (δ_m) must be satisfied at every demand site in the supply chain

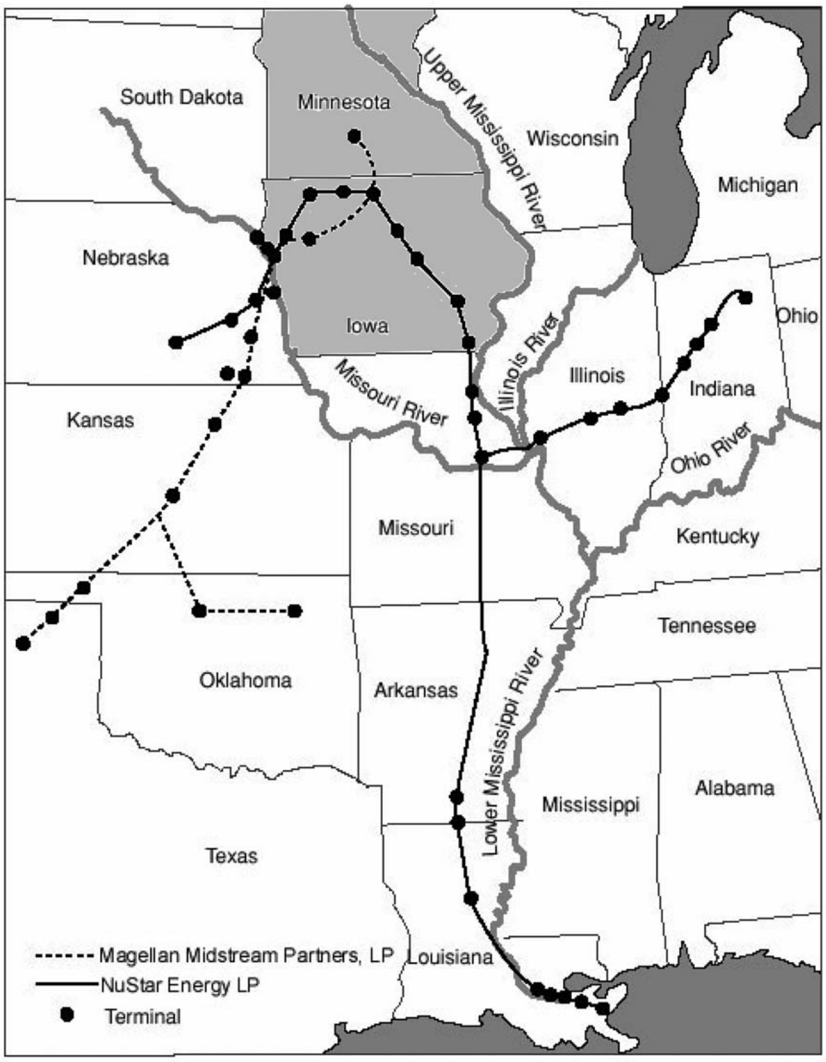

Figure 4. Existing ammonia pipelines in the United States.[25]

$$\sum_{d=1}^{D} y_{d,m} + \sum_{r=1}^{R} y_{r,m} \geq \delta_m \quad \forall m \tag{5}$$

Lastly, all decision variables must be nonnegative, as backwards flows are not allowed in the supply chain, and it makes no physical sense to built a plant with negative capacity

$$x, y \geq 0 \quad \forall d, m, p, r \tag{6}$$

Equations 1–6 provide physical constraints to the supply chain optimization.

To complete the optimization framework, an objective function is required. It is important for sustainable supply chains to consider both economic and environmental concerns. Using multiobjective optimization techniques, such as the epsilon constraint method,[26] objectives relating to both can be accounted for. First, an economic objective can be considered by examining the annualized cost of operating the supply chain

$$\begin{aligned}\text{cost} = &\sum_{r=1}^{R}\left(\sum_{u=1}^{U}\left(\frac{\rho_u}{\theta}\left(\frac{x_r}{\chi}\right)^{\gamma_u}\right) + \sigma x_r\right) + \sum_{r=1}^{R}\sum_{m=1}^{M}\tau_{r,m} y_{r,m} \\ &+ \sum_{p=1}^{P}\sum_{d=1}^{D}(\tau_{p,d} + \alpha_p) y_{p,d} + \sum_{d=1}^{D}\sum_{m=1}^{M}\tau_{d,m} y_{d,m}\end{aligned} \tag{7}$$

where ρ_u is the reference capital cost of a unit in the renewable plant, γ_u is the capacity exponent of that unit, θ is the scaled plant lifetime, using a 20-year NPV formulation with a 7% discount rate, χ is the reference renewable plant capacity corresponding to the reference capital cost, σ is the operating cost factor for a new renewable plant, $\tau_{i,j}$ are transportation costs of moving ammonia from i to j, and α_p is the cost of purchasing ammonia from conventional plant p. This is the overall supply chain cost, which consists of terms including the annualized capital cost of building new renewable ammonia plants, the operating costs of these new renewable plants, the cost of transporting ammonia through the supply chain, and the cost of purchasing ammonia from conventional plants, respectively. It is important to note here that a nonlinearity is present in the capital cost term due to economies of scale. The objective function also considers that the economies of scale may differ among units within the renewable plant; for example, electrolyzer units may not scale as well as the ammonia reactor.

An environmental objective is also considered by accounting for the annual amount of carbon dioxide produced from the ammonia supply chain

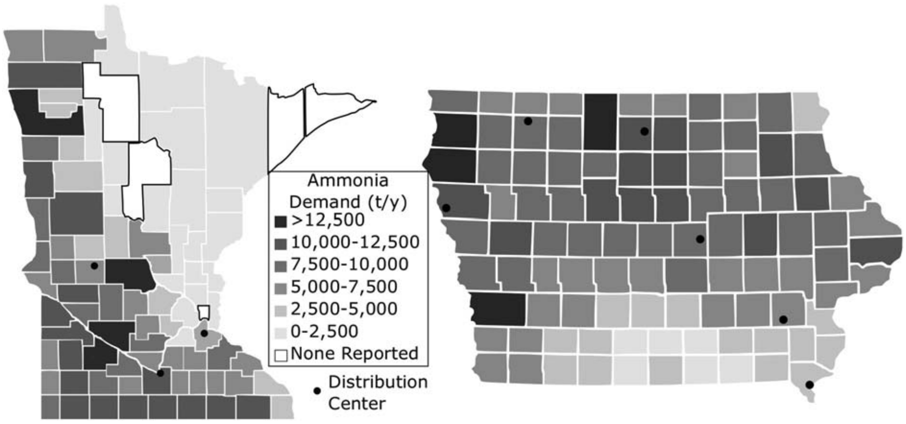

Figure 5. Ammonia demand and distribution centers in Minnesota (left) and Iowa (right).[28–30]

$$\text{emissions}=\sum_{p=1}^{P}\sum_{d=1}^{D}(\epsilon_{p,d}+\eta_p)y_{p,d}+\sum_{d=1}^{D}\sum_{m=1}^{M}\epsilon_{d,m}y_{d,m}+\sum_{r=1}^{R}\sum_{m=1}^{M}\epsilon_{r,m}y_{r,m} \tag{8}$$

where $\epsilon_{i,j}$ are the emissions resulting from transporting ammonia from i to j, and η_p are the emissions resulting from the production of ammonia at conventional plant p. These are the overall supply chain emissions, which consist of terms including the emissions resulting from transporting ammonia throughout the supply chain, as well as from conventional ammonia production, respectively. The emissions function assumes that all of the power required for renewable ammonia production is obtained from either direct or stored wind power, and as such, renewable ammonia production has no associated carbon emissions.

With the economic and environmental objectives defined, the supply chain optimization framework is complete. This formulation is a nonconvex nonlinear program (NLP) due simply to the capital cost term, as the capacity exponent γ_u will typically take values less than 1 due to economies of scale. The formulation could in theory be transformed to a mixed integer linear program (MILP) if only the economic objective is considered, as the economies of scale would dictate always building a plant to its maximum capacity if built. However, the presence of the second, environmental, objective, means that in some cases the optimization will decide to build new renewable plants that are smaller than what is allowed to decrease transportation emissions. The optimization model can be solved to global optimality for problems with a small number of variables or tight known variable bounds by, for example, using the BARON solver.[27]

Case Study Preliminaries

To demonstrate the utility of the proposed framework, it is applied to two separate case studies, analyzing the ammonia supply chains of Minnesota and Iowa, respectively. Note that the supply chain framework defined in the previous section allows for system boundaries as large or small as one would like. The choice of Minnesota and Iowa, is made because even though they are neighboring states, they have significant differences that make looking at each of the respective supply chains a worthwhile exercise as specified below. First, as shown in Figure 4, Iowa has more ammonia pipeline connections than does Minnesota. Because of this, there is also a greater number of distribution centers in Iowa, as shown in Figure 5. Figure 5 also shows agricultural ammonia demand at a county level for each state. This demand was calculated using crop planted area data for three major regionally grown crops: corn and wheat, which have a high demand for ammonia, and soybeans, whose demand is much less.[28,29] Reported data for the average ammonia consumption per area for each crop was then used to convert this agricultural use to an ammonia demand.[30] Looking at Figure 5, it is apparent that Iowa has a larger, more geospatially homogeneous demand for ammonia than Minnesota.

Ammonia can be purchased from any of the existing conventional ammonia plants shown in Figure 6[7] at a nominal market price of \$717/ton.[31] Depending on whether the existing plant uses coal or natural gas as its source for hydrogen, the related CO_2 emissions from purchasing this ammonia are 3.8 or 1.6 t CO_2/t NH_3, respectively.[32] For each plant, a maximum

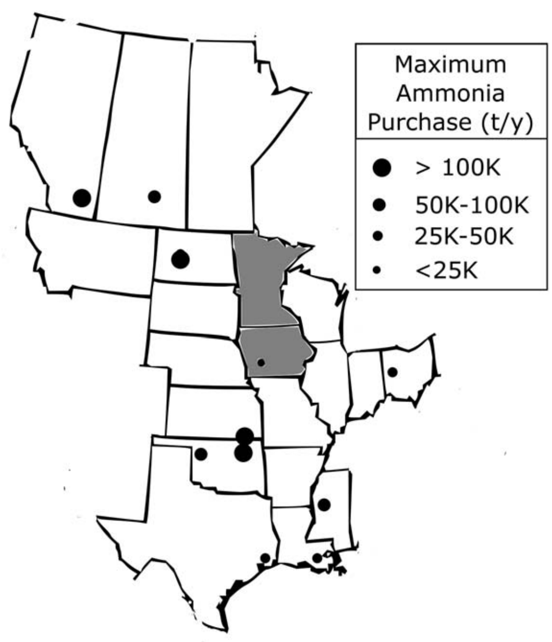

Figure 6. Existing conventional ammonia plants considered in this study, with Minnesota and Iowa highlighted in gray.[7]

Table 1. Maximum Purchases and Supply Chain Connectivity for Each Conventional Ammonia Plant Considered

Conventional Plant	Rail Connections	Pipeline Connections	Maximum Purchase (t/y)
Beulah, ND	Glenwood, Garner, Spencer, Sloan	N/A	150,000
Regina, SK	Glenwood, Garner, Spencer, Sloan	N/A	50,000
Medicine Hat, AB	Glenwood, Garner, Spencer, Sloan	N/A	300,000
Creston, IA	N/A	Mankato, Garner Spencer, Ft. Madison Washington, Marshalltown	10,000
Coffeyville, KS	N/A	Mankato, Sloan	100,000
Verdigris, OK	N/A	Mankato, Sloan	120,000
Woodward, OK	N/A	Mankato, Sloan	100,000
Yazoo City, MS	Rosemount, Ft. Madison, Washington, Marshalltown	N/A	50,000
Beaumont, TX	Rosemount, Ft. Madison, Washington, Marshalltown	N/A	30,000
Geismar, LA	Rosemount	Garner, Spencer, Ft. Madison, Washington Marshalltown	40,000
Lima, OH	Rosemount, Washington, Marshalltown	N/A	40,000

amount of ammonia allowed for purchasing was determined based on the capacity of each plant scaled down based on how far away such plant is from the area of interest, since conventional plants would presumably be supplying other areas and demands as well. Ammonia purchased from the conventional plants can be supplied to existing distribution by either pipeline, rail, or truck. Table 1 gives the maximum purchase parameters and transport connections for each conventional ammonia plant. Note that the maximum purchases given are for Minnesota, and Iowa maximum purchases are assumed to be 50% higher due to its larger demand. Truck transport is not included in this table, but is the default mode of transport between conventional plants and distribution centers if pipeline and rail transport are unavailable. Ammonia is then transported by truck from either distribution centers or new renewable plants to local demand sites, which in this case study are assumed to be cities located near the centers of each county with ammonia demand, as shown in Figure 5.

Truck transportation costs and emissions were determined assuming the use of diesel fuel with fuel economy of 2.13 km/L, a fuel cost of \$0.93/L, fuel emissions of 2.68 kg CO_2/L, a single tanker capacity of 17 t,[25] and a truck driver wage of \$22/h.[33] Driving distances and times were found using the Google Maps distance matrix API.[34] Pipe transportation costs were determined assuming a piping energy requirement of 185 kJ/kg,[25] an electricity cost of \$0.08/kWh, and emissions of 0.98 kg CO_2/kWh, the average from coal power plants.[35] An additional distance-based pipeline fee is added based on existing data adjusted for inflation.[25] Lastly, rail transport costs and emissions use the same fuel data as for truck transport, with a fuel economy of 204 km-t/L and an additional flat fee based on existing data adjusted for inflation.[25]

The candidate locations for new renewable ammonia plants are shown in Figure 7. These candidate sites are cities with nearby existing wind capacity:[36] this case study assumes that a new renewable plant would partner with this existing capacity rather than build new wind turbines, to avoid introducing additional capital costs in the economic analysis. It is further assumed that a maximum of 37% of the rated wind capacity could be used for the new ammonia plant, consistent with typical capacity factors for wind power, at a conversion rate of 1191 t/y/MW, a value obtained from runs of the pilot plant. For example, these parameters imply that a candidate location with a 15MW wind farm will be able to support a renewable plant no larger than 6610 t/y. It is important to note that for model generality, this capacity factor was assumed constant for all locations, although in reality it will be a function of both turbine design and location. From Figure 7, it is evident that Iowa also has a larger average maximum renewable plant size in comparison to Minnesota. Comparing Figures 5 and 7, it is easy to see the overlap between locations of high ammonia demand and high wind potential, presenting the possibility of ammonia production at a local scale rather than importing the ammonia from out of state.

Economic parameters for the new renewable plants are obtained from the pilot plant data obtained from the WCROC facility and are summarized below. From this facility, a total capital cost of \$2.6MM is obtained at a reference capacity of 26.28 t/y. Of this capital cost, 57% is from the ammonia reactor and related components, 28% is from the electrolyzer and related components, and the remaining 15% is from the air separation unit and related components. It is further assumed that a larger, more cost efficient electrolyzer is used in the new renewable plants in comparison to the pilot plant, giving a 25% cost reduction for this unit due to electrolyzer economies of scale for sizes up to 2MW. Beyond this scale-up, however, electrolyzer economies of scale are not as favorable as the rest of the plant,[37] and as such capacity exponents of 0.67, 0.67, and 0.85 are assumed for the ammonia, nitrogen, and hydrogen units, respectively. This capital cost is annualized using an NPV formulation that assumes a 20-year plant lifetime with 7% annual discount rate. In addition, an operating cost for operating the new renewable plant of \$308/t is applied that

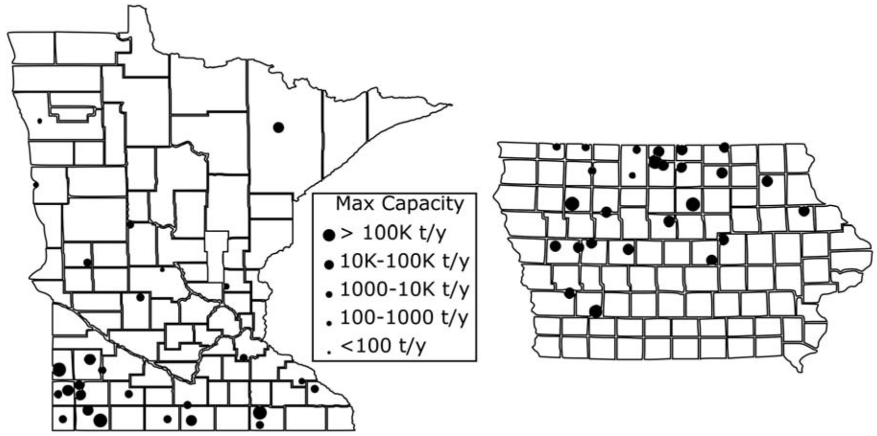

Figure 7. Candidate locations for new renewable ammonia plants considered in the study.[36]

takes into account energy costs ($294/t), labor, and maintenance ($14/t).

Results and Discussion

Base case results

For both the Iowa and Minnesota supply chains, the optimization model was solved using the BARON optimizer in GAMS. For the Minnesota supply chain, the model consisted of 2,522 variables and 152 constraints, while for the Iowa supply chain, the model consisted of 3,262 variables and 170 constraints. The model returned the economic optimal solution in 4.67 s for the Iowa supply chain and 2.64 s for the Minnesota supply chain. The low CPU-times can be attributed to the fact that the problem is mostly linear except for one concave objective, and that upper and lower bounds on all variables are known due to the mass balances within the supply chain. The model solved the problem to a 10^{-9} relative optimality gap using an Intel Core i7 3.40 GHz 64 bit processor. A tight optimality tolerance is used to ensure that all variables which should be zero are not small non-zero values in the solution; the fast solution times confirmed that this choice did not have a major effect on performance.

For the base case parameters, the annual cost of providing ammonia for the Minnesota supply chain in the economically optimal case was $426 MM/y, or an average consumer cost of $825/t NH_3. For the Iowa supply chain, the optimal annualized cost was $600 MM/y, or an average consumer cost of $827/t NH_3. The resulting supply chain emissions in the cost optimal case were $1.38*10^6$ t/y and $1.70*10^6$ t/y for Minnesota and Iowa, respectively. In both cases, the economic base case decided to build no new ammonia plants, and instead purchased all ammonia from conventional plants. The slightly higher average consumer costs in the Iowa supply chain are due to its higher demand, which needed to be met by purchasing ammonia from plants that were located further away from Iowa, incurring slightly higher transportation costs.

Figure 8 shows the base case economic optimal supply chains for Minnesota and Iowa. In both states, all of the available distribution centers are used to supply the state's ammonia demand. Although the Minnesota supply chain requires more in-state transportation than Iowa due to its fewer distribution centers, transportation costs take up about the same amount of the total costs, about 13%, for both states. This is because Iowa sees additional transportation costs due to requiring ammonia from further away conventional plants to meet its larger demand. While both states choose to purchase ammonia from the midwestern conventional plants in Iowa, North Dakota, Kansas, Oklahoma, and Ohio, the Iowa supply chain purchases extra ammonia from the southern plants in Louisiana and Mississippi, while the Minnesota supply chain instead uses the Canadian plants in Alberta and Saskatchewan.

The base case was further analyzed by applying the environmental objective function. For Minnesota, the environmentally optimal solution gave a supply chain cost of $620 MM/y, 46% more than the economically optimal cost, and emissions of

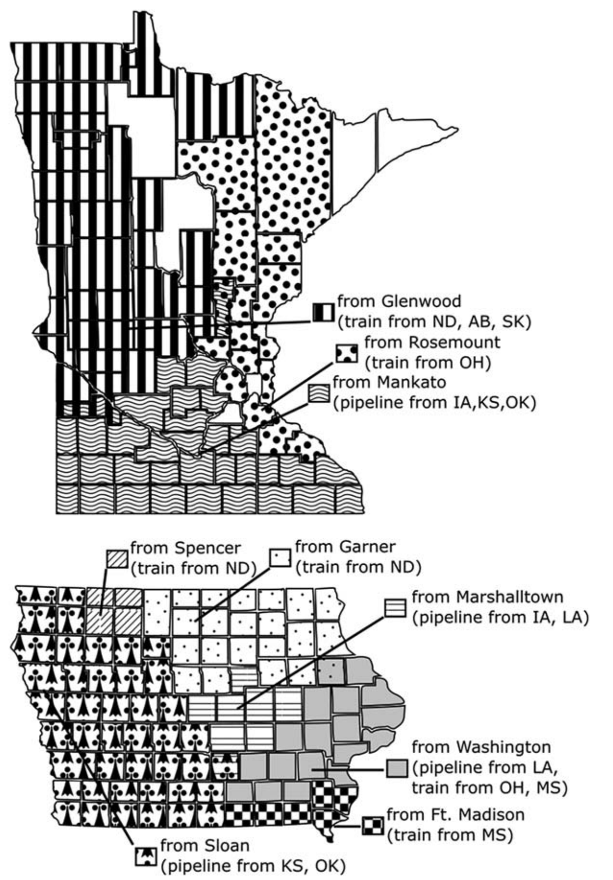

Figure 8. Base case economic optimal supply chains for Minnesota (top) and Iowa (bottom).

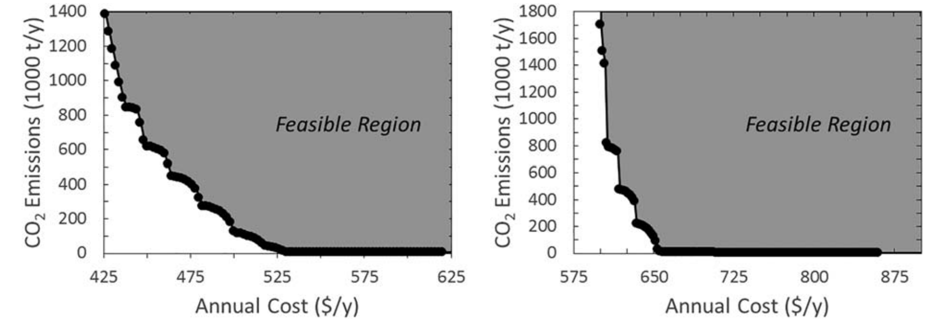

Figure 9. Pareto frontiers for supply chain costs vs. emissions for Minnesota (left) and Iowa (right).

6740 t/y. Averaged over the total ammonia demand, this equates to a consumer cost of \$1200/t NH_3 with related emissions of 0.0131 t CO_2/t NH_3. For Iowa, the environmentally optimal solution gave a supply chain cost of \$860 MM/y, 43% more than the economically optimal cost, and emissions of 4490 t/y. Averaged over the total ammonia demand, this equates to a consumer cost of \$1190/t NH_3 with related emissions of 0.00619 t CO_2/t NH_3. In both cases, the environmentally optimal solution returned a supply chain that obtained ammonia only from building new renewable plants, and these plants were highly distributed to minimize transportation, which is the only cause of emissions in this case. Additionally, the resulting emissions were three orders of magnitude lower in the environmentally optimal solution than in the economically optimal solution, implying that emissions from hydrogen production are the key source of emissions in the ammonia supply chain. As Iowa has more candidate locations that are close to the counties with high ammonia demand, the optimal emissions for Iowa are less than those of Minnesota. However, for both states, the emissions in the environmentally optimal case are multiple orders of magnitude smaller than the emissions in the economically optimal case. A pictorial representation of the supply chain solution for the environmentally optimal case is omitted here for brevity.

Using the results obtained from the purely economically or environmentally optimal solutions, a Pareto front comparing the trade-offs of these two objectives was obtained using the epsilon constraint method. The results are shown in Figure 9. Note that initially, the Pareto front for the Iowa supply chain drops at a steeper rate than that of the Minnesota supply chain. This indicates that renewable plants are closer to being cost competitive in Iowa than they are in Minnesota, a result of Iowa having larger existing wind plants, and as such, larger capacity candidate renewable plant sites. In both cases, the Pareto front (from left to right on Figure 9) first sees a region where a large amount of emissions reduction is achieved with relatively little cost increase, indicating a switch from purchasing ammonia from conventional sites to building new renewable plants. However, at higher costs, only a very small emissions reduction is occurring for a larger cost increase and the Pareto front is essentially flat. At this point, no more ammonia is being purchased from conventional plants, and the emission reductions seen are a result of building smaller scale renewable plants in a distributed fashion, reducing emissions from in-state transportation. Similar arguments account for the non-smooth nature of the Pareto front; jumps in cost occur when emissions are reduced by building a new renewable plant at its maximum capacity, while more gradual cost changes indicate that emissions are reduced by changing how ammonia is transported.

Carbon tax sensitivity

Multiobjective optimization showed that starting at the economically optimal solution, there is potential for a high amount of emissions reduction for little additional cost. This implies that economic incentives, such as a carbon tax, may be effective in promoting new renewable plants to be present in the economically optimal solution. This is tested by optimizing a new function which takes into account the supply chain costs previously considered, as well as the supply chain emissions:

$$\text{new cost} = \text{cost} + \zeta(\text{emissions}) \tag{9}$$

where ζ is the value of the carbon tax. Note that analyzing the carbon tax using this formulation has the practical effect of combining the two objectives examined in the base case into a single, weighted objective, with weights dependent on the value used for ζ.

The results of this optimization are shown in Figure 10. In this figure, notice that a carbon tax is immediately effective at curbing emissions for the Iowa supply chain. However, the Minnesota optimal supply chain is not affected from a carbon tax until a value of \$25/t. This is indicated by a jump down in emissions between carbon taxes of \$20/t and \$25/t, and in general, a jump in emissions indicates the optimal solution deciding to replace conventional ammonia with a newly built renewable ammonia plant at higher carbon tax. Overall, the carbon tax has a greater impact on the cost of the Minnesota supply chain, with a cost increase of \$83 MM/y, or 19% occurring from a \$100/t carbon tax, compared to only a \$55 MM/y or 9% cost increase in Iowa from the same carbon tax. Additionally, these results show that a reasonable carbon tax can be effective at reducing ammonia supply chain emissions and providing incentives to build new renewable ammonia plants: at a carbon tax rate of \$35/t, similar to what has been proposed or implemented in other OECD countries, emissions are reduced by 76 and 39% in Iowa and Minnesota, respectively. Again, the reason for these differences is economies of scale: fewer economic incentives are required to make the larger candidate plants in Iowa attractive than are necessary to make the smaller candidate plants in Minnesota attractive.

Ammonia price sensitivity

One of the key parameters in determining the economic feasibility of renewable ammonia is the cost of conventional

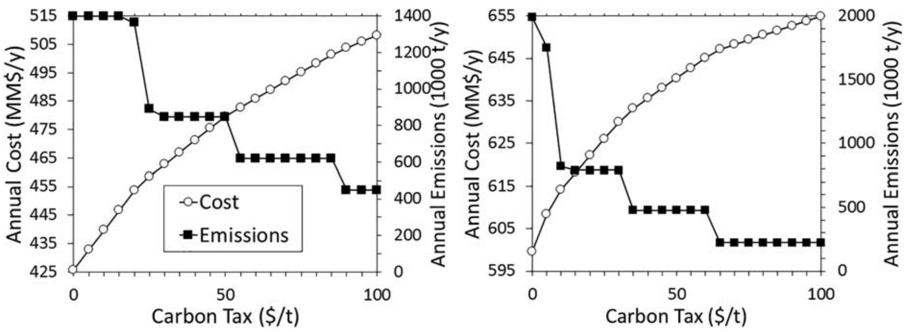

Figure 10. Effect of a carbon tax on annual cost and emissions of economic optimal supply chain for Minnesota (left) and Iowa (right).

ammonia. Ammonia costs in the upper Midwest can vary wildly from year to year, with costs ranging from $450/t to $900/t since 2008.[38] Thus, it is instructive to analyze the effects of ammonia costs on the supply chain optimization. To perform this analysis, the total annual supply chain costs are broken into three categories: the costs of purchasing ammonia from conventional plants, the costs of building and operating new renewable ammonia plants, and the costs of transporting ammonia throughout the supply chain. The effects of ammonia cost on these supply chain costs are shown in Figure 11.

From Figure 11, it is clear that several distinct "regions" appear in the parameter space as ammonia cost is varied. The boundaries between these regions are where discontinuities in the three categories of costs occur. Each of these discontinuities represents a change in the optimal supply chain such that an additional renewable ammonia plant is built. For example, the results of the Iowa supply chain indicate that one new renewable ammonia plant is built at prices of $745/t or higher, while no new plants are built at prices of $740/t or lower. Note that as ammonia prices increase and more renewable plants are selected to be built, the transportation costs also decrease. This is an indirect result of selecting ammonia sources that are closer to the final demand sites, instead of purchasing ammonia from far away conventional plants.

Figures 12 and 13 show the supply chain results for the different solution regions for Minnesota and Iowa, respectively. Note that the results for the region where no renewable plants are built are the base case results; these results were shown previously in Figure 8. As keeping transportation at a minimum also minimizes the supply chain costs, new renewable plants replace the nearest distribution center as the source for ammonia. For example, when comparing the Minnesota supply chains with zero and one new ammonia plant built, note that the distribution center in Rosemount is no longer used when the new plant is built. In fact, many of the counties that were receiving ammonia from Rosemount when no plants are built instead receive ammonia from the newly built renewable plant in Dexter when ammonia prices are higher and it is selected to be built.

Monte-Carlo analysis

While the carbon tax and ammonia price are important parameters affecting the optimal supply chain, they are not the only parameters which have a large impact. In this section, the effects of four key parameters, which include both the carbon tax and ammonia price as well as the electrolyzer scaling exponent and the conversion factor between available wind capacity and renewable plant maximum size, are explored in a Monte Carlo analysis. Such an analysis gives insights on the robustness of the supply chain with respect to different economic and weather conditions which may be present. In particular, the frequency of building new renewable plants and purchasing from conventional plants is determined. The distributions used for each the four parameters are as follows: first, for the ammonia price, a Gaussian distribution is used based on the mean and standard deviation from the historical data since 2008.[38] The wind power to maximum plant size conversion factor is also varied by a Gaussian distribution with its mean at the base case value and a standard deviation value of 20% of the mean. For carbon tax, an exponential distribution is considered with a mean value at a reasonable $20/t tax, and the most likely value at the status quo of no carbon tax. Lastly, the electrolyzer capacity exponent varies uniformly from a lower bound of 0.67, where the unit scales as well as all others, to an upper bound of 1, where the unit does not scale at all. For each supply chain, Monte Carlo random sampling using the given distributions is performed and the optimal supply chain is found by solving the optimization using the

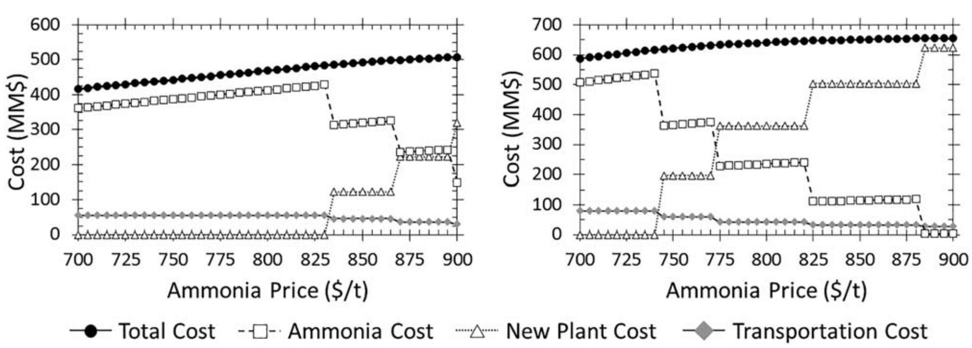

Figure 11. Effect of ammonia prices on economic optimal supply chain costs for Minnesota (left) and Iowa (right).

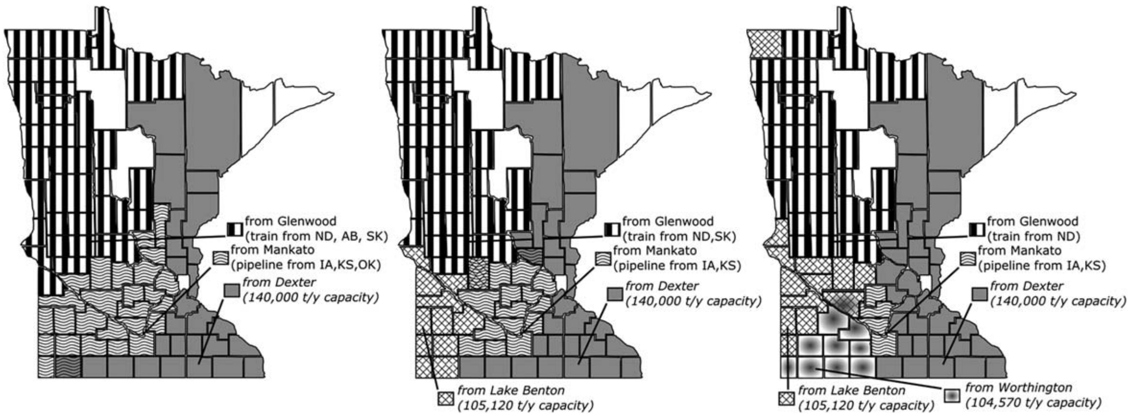

Figure 12. Minnesota economic optimal supply chain for cases where 1 (left), 2 (middle), and 3 (right) new renewable plants are built, with renewable plants in italics.

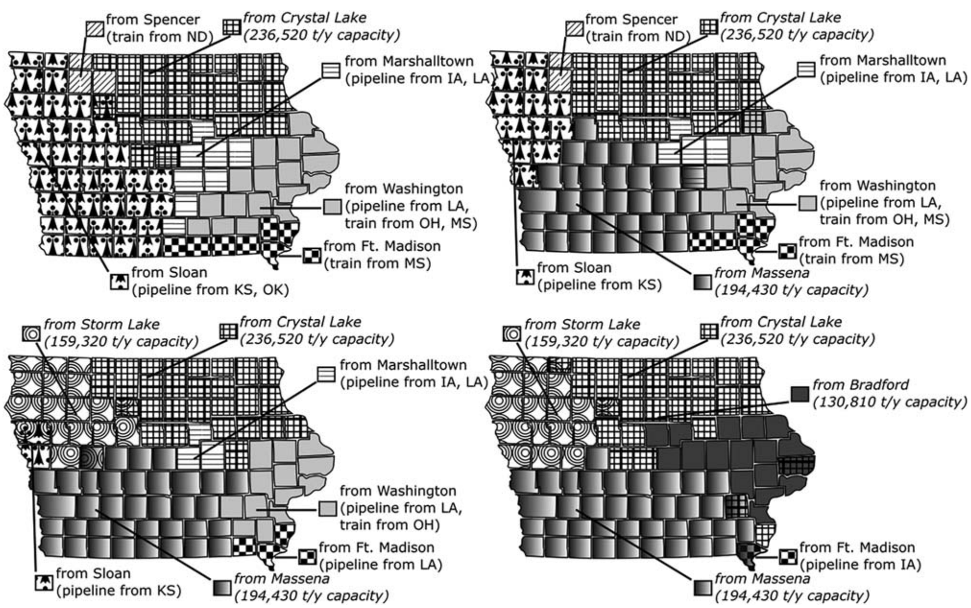

Figure 13. Iowa economic optimal supply chain for cases where 1 (top left), 2 (top right), 3 (bottom left), or 4 (bottom right) new renewable plants are built, with renewable plants in italics.

randomly generated parameters. This process is repeated 6000 times for each supply chain to adequately explore the parameter space.

The results of the Monte Carlo analysis show that neither renewable plants nor conventional plants are 100% robust, as shown in Figure 14. In fact, there exist scenarios where no renewable plants are used, as well as those where no conventional plants are used. For Iowa, no renewable plants are built 44% of the time while no purchases from conventional plants are made 9.7% of the time. For Minnesota, the results favor conventional plants more, as no renewable plants are built 72% of the time while no purchases from conventional plants

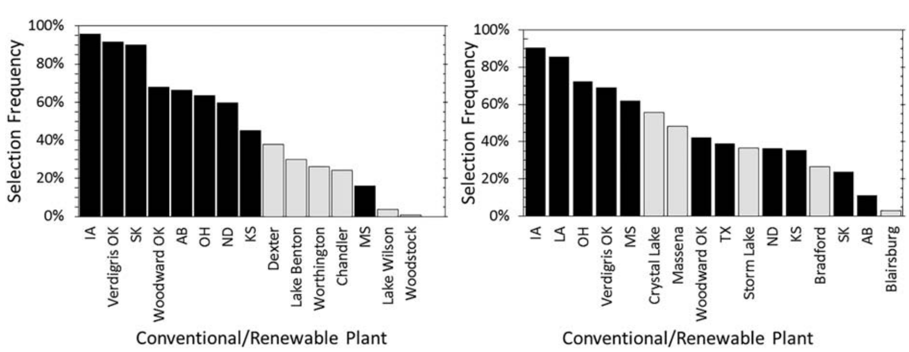

Figure 14. Frequency of conventional (black) and renewable (gray) plants being selected in supply chain during Monte Carlo analysis for Minnesota (left) and Iowa (right).

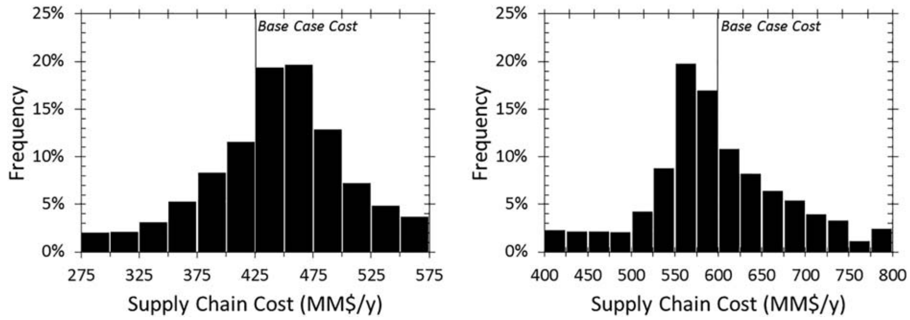

Figure 15. Histogram of annual supply chain costs from Monte Carlo analysis for Minnesota (left) and Iowa (right).

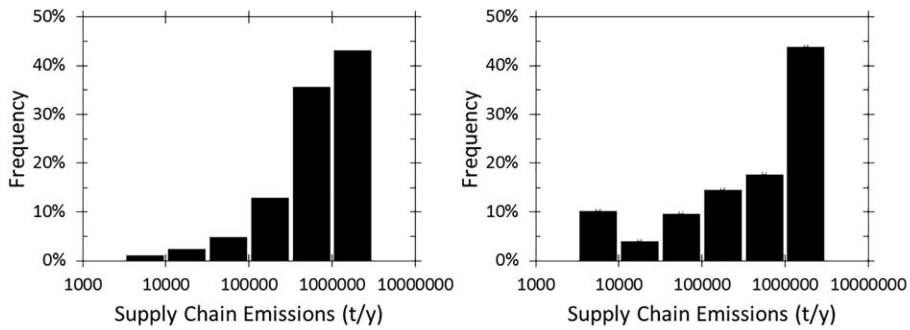

Figure 16. Histogram of annual supply chain emissions from Monte Carlo analysis for Minnesota (left) and Iowa (right).

are made only 4.3% of the time. Again, the reason for this is scale: the largest candidate renewable plant in Iowa, located in Crystal Lake, is selected the most, 56% of the time. However, the largest renewable plant in Minnesota, located in Dexter, is almost 100,000 t/y smaller than the Crystal Lake plant, and as such is only selected 38% of the time.

The observed distributions of costs and emissions are shown in Figures 15 and 16, respectively. Emissions are plotted on a log scale since the results vary over orders of magnitude depending on how many renewable plants are selected. Interestingly, the average cost seen is higher than the base case cost for the Minnesota supply chain but lower in the Iowa supply chain. This is likely a result of the Iowa renewable plants being more competitive than Minnesota renewable plants. As such, certain parameter values may result in a new renewable plant being built in Iowa but not in Minnesota, and thus the relative cost per ton of ammonia will be lower in Iowa but higher in Minnesota. This explanation is further supported by the emissions distributions, as Minnesota had a higher likelihood of a high emission supply chain than Iowa.

Analysis of smaller scale systems

The case study results discussed thus far explore which, if any, renewable plants should be built given certain economic and demand parameters. The answers that have been obtained, not surprisingly, say that the largest scale candidate plants are the most optimal to build since they have lower capital costs per unit capacity. However, the idea of distributed ammonia was introduced with the desire to produce this chemical at a smaller, more distributed scale to take advantage of the geospatially distributed wind supply and agricultural demand. The framework developed in the article also allows for analysis of the reverse question; that is, given a specific size of renewable plant to build, what economic parameters are required to make such a plant economically competitive in the supply chain. This analysis allows us to identify policy or technology targets that should be met to make smaller scale renewable ammonia plants economically competitive.

For this analysis, candidate renewable plant capacities were set to a maximum value of the specific capacity that was being analyzed. Three economic parameters were then separately analyzed: the cost of purchasing ammonia from conventional plants, the cost of a carbon tax, the base case plant capital cost, and the plant's capacity exponent. These parameters are gradually increased (in the case of ammonia cost and carbon tax), or decreased (in the case of capital cost) until the

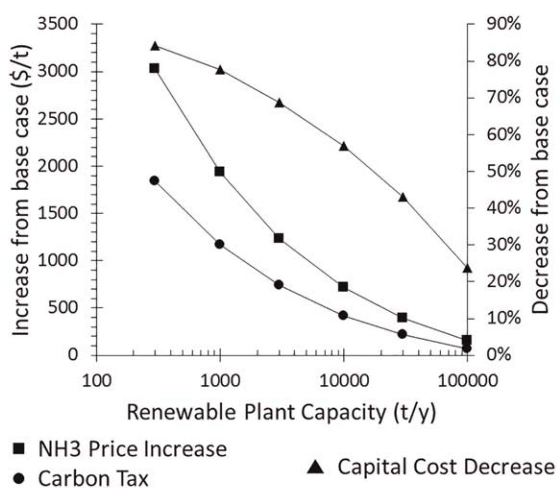

Figure 17. Required changes in parameters for renewable plants of a certain scale to be economically optimal.

optimization returns a solution where a renewable plant is built. This is repeated over various ammonia plant capacities of interest, including scales as large as 100,000 t/y (ammonia to provide to 1.84 million acres of corn, or 2% of all US corn fields) to as small as 3,000 t/y (ammonia to provide to 5500 acres of corn, or about 3–4 large family farms). The results of this analysis are shown in Figure 17, where only single lines are shown as the results from Minnesota and Iowa are not different enough to be distinguished on the plot.

The results shown in Figure 17 give good insight of the issues of building small scale, distributed plants. It is apparent that, at the scale of 100,000 t/y, renewable ammonia plants are not that far from being economical. For a plant of this scale to be competitive, only a 20% increase in ammonia cost, a 22% decrease in base plant capital costs, a $64/t carbon tax, or some combination of the three, is required. However, at a 30,000 t/y scale, these metrics become increasingly less achievable: a 55% increase in ammonia cost, a 43% decrease in capital costs, or a $218/t carbon tax is required. The results again show the importance of economies of scale for chemical plants, as plant economics very quickly become restrictive when considering smaller scales. However, it is also important to note that the smallest plants may actually perform slightly better than this analysis shows since ammonia demand is only determined at the county level, whereas the smallest plants would serve a smaller demand and have near zero transportation costs.

Conclusions

In this article, a novel formulation for ammonia supply chain optimization was presented that considers both the existing conventional production technology, as well as a newly developed renewable production technology. Such a framework allows for meaningful comparison of the two technologies in their ability to meet existing ammonia demands considering both economic and environmental objectives. It is important to note that the framework provided here is generic: while the studies presented analyze wind-powered renewable ammonia and agricultural ammonia demand, it is also possible to use, for example, solar power and consider fuel or chemical industry demands.

We then applied the developed framework to the ammonia supply chains in the states of Minnesota and Iowa, respectively. Analyzing these supply chains separately gave insights on the effects of how the number of distribution centers or overall demand size affect the supply chain results. Perhaps unsurprisingly, the key conclusion that was obtained from the separate analysis was the importance of scale: economies of scale are essential for renewable plants to be cost-competitive, and the smaller candidate plants located in Minnesota do not perform as well as the larger candidate plants in Iowa. However, the analysis shows that renewable plants have the potential to be cost-competitive under the right economic parameters, as the largest possible renewable plant was selected 71% of the time under a Monte Carlo sensitivity analysis. This result in itself shows that the new renewable ammonia technology developed is a promising one which holds potential for growth, improvement, and successful breakthrough into the market.

The framework presented here allows for long term planning of the ammonia market and supply chain. However, one such potential for improvement of the renewable ammonia technology involves moving down a level and focusing on the shorter-term scheduling and control of the system. Because the renewable ammonia system relies on stochastic renewable energy to power it, cost savings may be achievable by intelligent scheduling and control of the renewable ammonia system. Performing this scheduling optimization and using the results to better inform the supply chain decision making is a promising avenue of future research that will be pursued in future work.

Acknowledgments

Financial support from the Minnesota Environment and Natural Resources Trust Fund as recommended by the Legislative-Citizen Commission on Minnesota Resources, and MnDRIVE, an initiative of the University of Minnesota, is gratefully acknowledged.

Notation

Sets

$d \in \{1,\ldots,D\}$ = ammonia distribution center sites
$m \in \{1,\ldots,M\}$ = ammonia consumption sites
$p \in \{1,\ldots,P\}$ = conventional ammonia production sites
$m \in \{1,\ldots,R\}$ = renewable plant candidate sites
$u \in \{1,\ldots,U\}$ = renewable plant operating unit

Parameters

α_p = cost of purchasing ammonia from site p (\$/t)
γ_u = capacity exponent for unit u
δ_m = ammonia demand at site m (t/y)
$\epsilon_{i,j}$ = carbon emissions from transporting ammonia from site i to site j (t CO_2/t NH_3)
ζ = carbon tax (\$/t CO_2)
η_p = carbon emissions from producing ammonia at site p (t CO_2/t NH_3)
θ = scaled plant lifetime y
ξ_p = maximum purchase of ammonia from conventional site p (t/y)
ξ_r = maximum capacity of new renewable ammonia plant built at site r (t/y)
ρ_u = reference capital cost of renewable plant unit u (\$)
σ = annual renewable plant operating cost per capacity (\$/t)
$\tau_{i,j}$ = cost of transporting ammonia from site i to site j (\$/t)
χ = reference renewable plant capacity (t/y)

Decision Variables

x_r = new renewable plant capacity built at candidate site r (t/y)
$y_{i,j}$ = ammonia transported from site i to site j (t/y)

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