DISTRIBUTED MANUFACTURING FOR ELECTRIFIED CHEMICAL PROCESSES IN A MICROGRID

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Abstract

To alleviate the greenhouse gas emissions by the chemical industry, electrification has been proposed as a solution where electricity from renewable sources is used to power processes. The adoption of renewable energy is complicated by its spatial and temporal variations. Millions of dollars might be saved if electrified processes can be designed to adapt to these variations. To address this challenge, we investigate the potential of distributed manufacturing of electrified chemical processes installed in a microgrid. We propose an MILP (Mixed Integer Linear Programming) model for locating and designing modular electrified plants and transmission lines in a microgrid. The proposed model has three-time scales which include single-time investment decisions, monthly decisions, such as transportation of chemicals to meet customer demand, and hourly decisions, such as chemical production, mode switching, and power flow. The model is tested using a case study with 5 candidate locations in Western Texas. A bi-level decomposition algorithm is developed which can obtain a solution within 1.4% time of solving the MILP model while maintaining an optimality gap of 0.042%. The optimal solution can locate the chemical plants such that the plants are operated to take advantage of the spatial and temporal variations of renewable output and electricity price.

Keywords

Electrification, Distributed Manufacturing, Multiscale Integration

Introduction

Chemical industries are a major source of greenhouse gas emissions and are responsible for 7% of global greenhouse emissions (Tickner et al., 2021) as they are mostly powered by the combustion of fossil fuels. To solve this problem, electrification of the chemical industry is a solution that is currently being explored by researchers across the world. Electrification helps decarbonize the chemical industry and move from fossil fuels to renewable energy sources such as solar and wind. Electrification can be done in different parts of the process including reaction and separation. A number of works have been done on electrification focusing on the optimization of process scheduling and design such as (Kelley et al., 2022), (Allman & Daoutidis, 2018), (Wang et al., 2021), (He et al., 2021), (Guerra et al., 2019), (Demirhan et al., 2019) and (Cooper et al., 2022).

Distributed Chemical Manufacturing (DCheM) aims to improve chemical process industries by developing modular process plants, which take advantage of distributed resources and/or address distributed environmental problems. DCheM paves way for the introduction of numerous new process technologies and simultaneously supports and enables energy and environmental sustainability while reducing transportation costs. Modular processes increase the flexibility in dealing with the variability of conditions. Work has been done in this field, such as (Sampat et al., 2021), (Lara & Grossmann, 2016), and (Palys et al., 2019).

While work has been done on the design and optimization of electrified plants, one of the areas which can be explored more is the spatial features of such plants as renewable resources such as wind and solar vary with location. While some research has been done on the supply chain optimization of a particular set of chemicals produced by electricity such as (Ochoa Bique & Zondervan, 2018), (Welder et al., 2018) and (He et al., 2021), these models do not consider the monthly demand variability or in some cases the hourly variability.

In this paper, we address this gap, where we model a network of plants and power generating units with three-time scales, single-time, monthly, and hourly. The problem is considered under the context of a microgrid, which typically consists of a network of low voltage power generating units, storage devices, and loads capable of supplying a local area such as a suburban area, industry, or any commercial area with electric power and heat (Mahmoud et al., 2014). The objective of this research is to design a network to facilitate DCheM for electrified chemical processes with the power demand satisfied by renewable sources as well as power from a utility grid coordinated by a microgrid operator by using an MILP (Mixed Integer Linear Programming) model. The major contributions of this paper are listed below:

- The proposed model encompasses three-time scales taking into account investment decisions, as well as monthly decisions and hourly decisions incorporating them into the same model and thus capturing temporal variations as well as spatial variations in all time scales.
- The model incorporates both the microgrid (generating units and transmission lines) and chemical plant expansion in a single model. Therefore, the tradeoffs between the transportation of chemicals and the transmission of power are considered.
- The size of the model can easily exceed millions of variables. We develop a bi-level decomposition method to solve the model efficiently while maintaining a small optimality gap.

Problem Statement

We are given a set of candidate locations. At each location, we can set up at most one modular chemical plant and/or multiple power-generating units. Modular chemical plants can be selected from several given technologies that involve electrochemical processes. For each plant, we are given the chemicals involved, the associated electrochemical reactions under different operating modes, and the equations to determine the power requirements. The modular power generating units are all renewable-based like solar panels and wind turbines. The wind speeds for the wind turbines and the solar radiation for the solar panels for several historical years are given on an hourly basis. Transmission lines can be installed between any two different locations or between any of the locations and the utility grid whose location is predetermined. The time span of our problem is a given year.

Raw materials are obtained from suppliers with fixed locations and transported to the installed chemical plants. The required chemicals are produced in the plants and transported to consumers in certain given locations. The electrochemical reactions in the plants consume the power obtained through the connected transmission lines. The consumed power can come from the installed generating units. In addition, when the microgrid produces excess electricity, the excess electricity can be sold to the utility. On the other hand, the microgrid operator has the option of purchasing electricity from the utility grid as well. The monthly demand forecasts for each chemical for each of the consumers are also given. In addition, we are also given the resistance and inductance of the candidate transmission lines, the electricity price at each hour, the variable transportation costs, the cost of capital, and the cost of different chemicals. We are also given the limits on production rates in different plants, power transmission, and power generation of the generating units.

The proposed MILP model makes decisions across three-time scales: investment decisions at the beginning of the time horizon, monthly delivery of the chemical products to the customers as well as the monthly purchase of raw materials, and hourly operating decisions of chemical plants, power generating units and power through transmission lines. To simplify the problem, we consider one year of operating decisions. The investment decisions include (a) which chemical plants and power generating units to install and the locations to install them, (b) which transmission lines should be installed. The monthly decisions include (a) the amount of each chemical sold from each plant to each consumer on a monthly basis, (b) the amount of each chemical purchased or outsourced from other sellers. The hourly operating decisions include (a) The amount of power produced by the generating units, (b) the power flow and power loss of all the installed transmission lines, (c) the amount of each chemical produced in each plant, (d) the amount of net electricity purchased/sold to the utility. There is a monthly demand for each consumer and a penalty of twice the price is paid for the part of the demand not met.

As an illustrative example, in the region considered as shown in Figure 1, we are given three candidate locations denoted by rectangles. Three modular technologies including chemical plants, wind turbines, and solar panels are given with the maximum number of each technology that can be installed being one. We can install at most one chemical plant, and/or multiple solar panels, and wind turbines in each of these candidate locations. Also, in the region shown, there are 2 consumers and 2 suppliers of raw materials and a utility grid whose locations are known. Transmission lines can be installed between any two different locations and between any of the locations and the utility grid. A solution to the problem is shown in Figure 2.

In the solution, one chemical plant is placed at R1, one solar panel at R3, and one wind turbine at R2 to meet the demand of the consumers most economically with appropriate transmission lines connected.

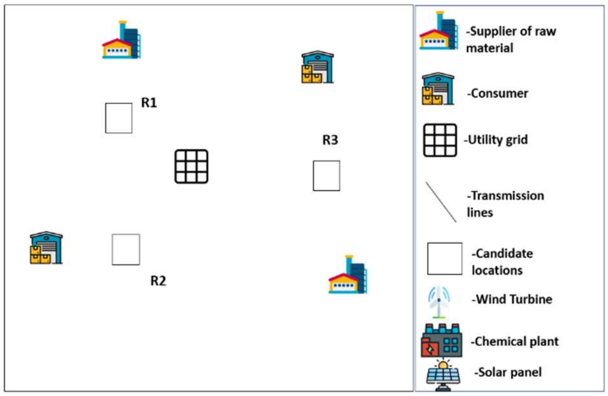

Figure 1 - Region representation

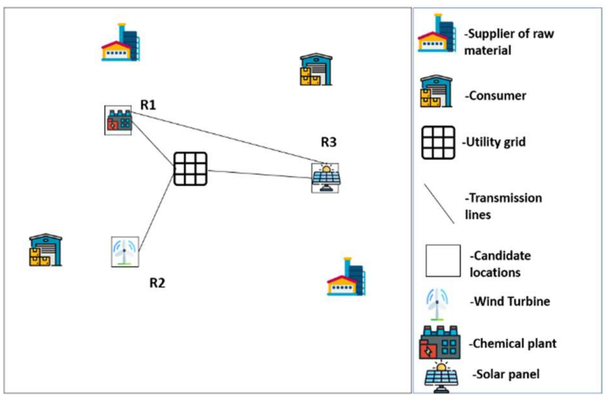

Figure 2 - Solution representation

MILP Formulation

In a full-scale model, there will be variables associated with all the 365 days. To reduce the number of variables while preserving the information in the data associated with the 365 days, 5 representative days are chosen for each month by applying a k-means clustering algorithm on the normalized solar and wind power output, and electricity prices for 3 years. Figure 3 is a representation of the various time scales of the decisions.

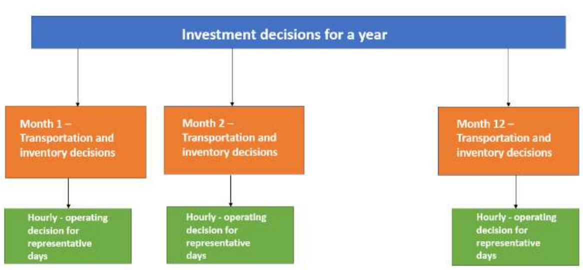

Figure 3 - Time representation

A succinct representation of the MILP formulation is shown in Equations (1)-(5). Integer variables y represent the investment decisions. Continuous variables x represent the monthly decisions for each month t. Continuous variables w and binary variables z represent the hourly decisions for each hour s on representative day k of month t. The formulation can be written as follows:

$$\text{Max } c^T y + \sum_{t=1}^{12} d_t^T x_t + \sum_{t=1}^{12} \sum_k \sum_s h_{t,k,s}^T w_{t,k,s} \quad (1)$$

Subject to:

$$Ay \leq b \quad (2)$$

$$Dx_{t-1} + \sum_k \sum_s E_{t,k,s} w_{t,k,s} = Fx_t \ \forall t \quad (3)$$

$$G_{t,k,s} y + Hw_{t,k,s} + Jz_{t,k,s} \leq g_{t,k,s} \ \forall t,k,s \quad (4)$$

$$Lw_{t,k,s} + Mz_{t,k,s} \geq Pw_{t,k,s-1} + Qz_{t,k,s-1} \ \forall t,k,s \geq 1 \quad (5)$$

Equation (1) represents the objective which is to maximize the total profit for a year. Equation (2) represents the constraints on the investment decisions, i.e., constraining the maximum number of each type of unit installed at each location. Equation (3) represents the monthly constraints such as the mass balance of the chemical inventory, transportation of the chemicals from the suppliers to the installed plants, and from the plants to the customers, and demand satisfaction. Equation (4) represents the constraints connecting the investment decisions and the hourly operating variables to enforce that a plant or transmission line can only be operated if it has been installed. Equation (5) represents the constraints only with hourly operating variables like mode transition constraints, stochiometric constraints, and power loss constraints for each hour.

In order to model the power flow through transmission lines, we apply the DC power flow model with losses for which we assume that the difference in voltage angles between 2 locations is very small using big-M formulation of DC power flow equation with a piecewise linear approximation of the quadratic power loss (Ahlhaus & Stursberg, 2013). The MILP model is optimized for a time scale of a year to determine the optimal investments.

Case Study

We implement the MILP model on a case study in Western Texas with there are 5 candidate locations whose coordinates are known. We are given three 1500 KW solar panels, three 100KW wind turbines, modular chlorine plants operating in 3 modes, and 12 kV transmission lines. We have also been given the location of the utility grid and the location of 3 consumers/suppliers.

The chlorine plant operates in 3 modes - standard cathodes (STCs), oxygen depolarized cathodes (ODCs), and shut down. The reaction with STC producing H_2 as by-product is: 2 NaCl + $2H_2O \rightleftharpoons$ 2NaOH + Cl_2 + H_2. The net reaction of the chlor-alkali electrolysis using an ODC is: 2NaCl + H_2O + $0.5O_2 \rightleftharpoons$ 2NaOH + Cl_2. The energy requirement and the capacity of the chlorine plant are obtained from Brée et al., (2019). The monthly demand data is randomly generated based on the capacity of the plant. The capital costs are estimated using ASPEN with fixed capital added for mode switching. The fixed capital cost is amortized for a year. We assume that the plant remains in one mode for at least 2 hours after switching to it in a day.

The power output for the wind turbines and solar panels at the candidate locations for 3 historical years as well as the capital costs of these power generating units are obtained from the software SAM (System Advisor Model) after obtaining the weather-related data from NREL (National Renewable Energy Laboratory) website. The electricity price for west Texas for 3 historical years is obtained from the website Energy Online ("ERCOT: Real-Time Price - LCG Consulting," n.d.). The electric properties of transmission lines such as resistance and inductance are obtained from the DERCAM (Distributed Energy Resource Customer Adoption Model) (Deforest et al., 2018).

Results

The proposed MILP model is implemented in Julia/JuMP and solved using Gurobi version 9.0.3. The MILP has 632,514 continuous and 86,565 integer (86,550 binary) variables and 2,737,439 constraints. The MILP model is solved on a PC laptop Intel (R) Xeon (R) W-1195M CPU with 16 x64- based processors and 128 GB 2.61 GHz memory with a time limit of 36,000 secs. At the time limit, it returns a solution with an MIP gap of 0.05%. The profit obtained is 2.6221 M $.

Because of the large amount of time taken to run the entire MILP model, we propose a bi-level decomposition algorithm as shown in Figure 4

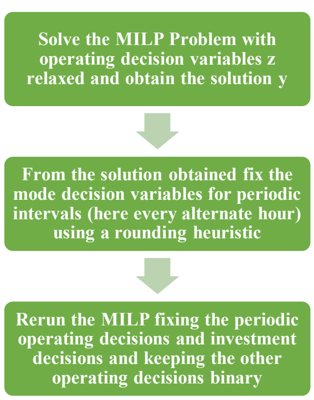

Figure 4 - Bilevel Decomposition Algorithm

In the first step which gives an upper bound, we obtain an optimum objective profit of 2.6229M$ in 509 seconds with an MIP gap of 0.56%, and the optimum configuration (investment decisions) which is the same as that obtained in the optimal investment decisions obtained from solving the full MILP model. In the second step, we deduce the mode decision variables for periodic intervals. In the third step which gives a lower bound and a feasible solution, we get an optimal profit of 2.6218 M$ in 11 seconds with an optimality gap of 0.042%.

Split of Profit

The split of the profit is shown below.

Table 1. Profit and cost breakdown

Split up of profit (for a year)	Cost/Revenue in M $
Net revenue from materials	3.17
Net transportation cost	0.036
Net profit from electricity	0.23
Total fixed operating cost	0.14
Total capital cost	0.60

An important observation from the split up of the profit is that the materials (raw materials and products) are the highest contributor to the profit followed by the total capital cost. The profit from the electricity makes a considerable contribution to the profit and thus the location of the plant and the power generating units could influence the profit.

Optimal Configuration

Figure 4 is a representation of the optimal configuration obtained from the MILP model. r1, r2, r3, r4, and r5 represent the candidate locations, ru represents the location of the utility grid while, j1, j2, and j3 represent the location of 3 consumers/suppliers. In the optimal configuration, one plant, three solar panels, and three wind turbines are installed at location r2, and 9 transmission lines are placed between r2 and ru.

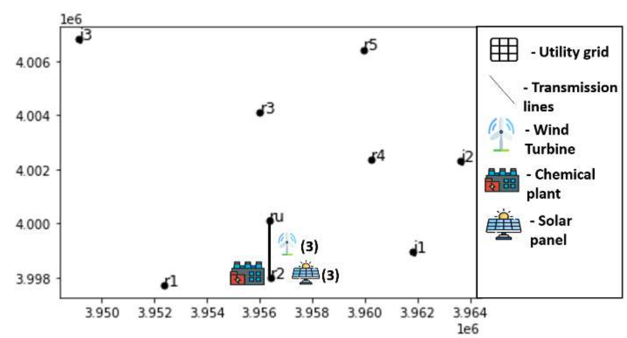

Figure 5 - Optimal configuration

Trends Discovered

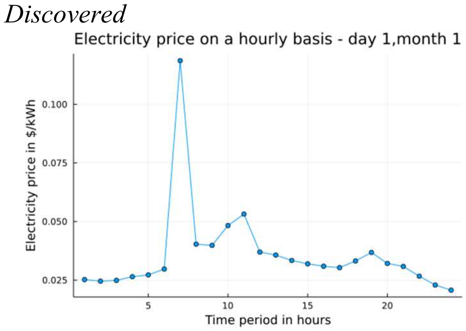

Figure 6 – Graph representing the electricity price

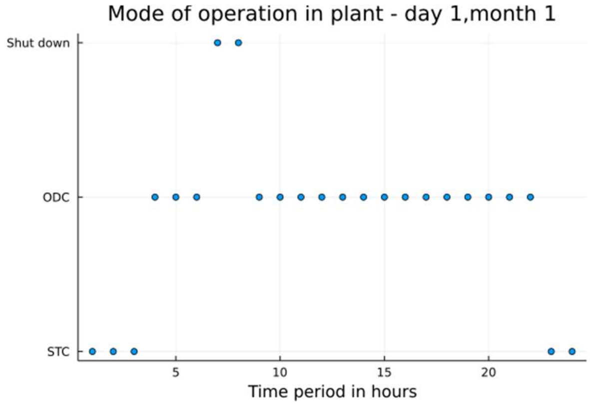

Figure 7 – Graph representing the mode decision

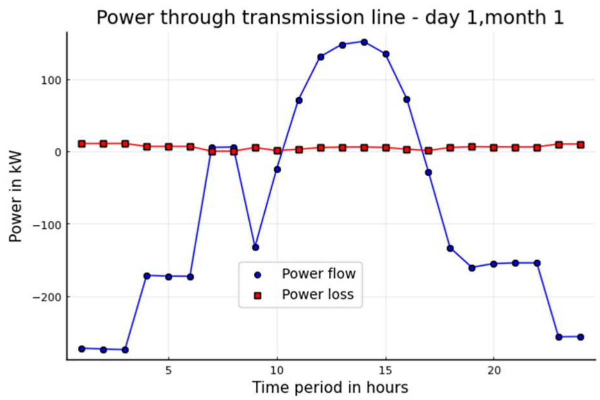

Figure 8 – Graph representing power flow and power loss through a transmission line

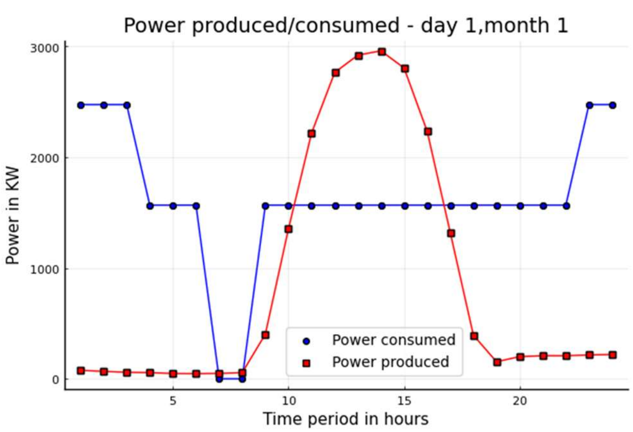

Figure 9 – Power produced or consumed

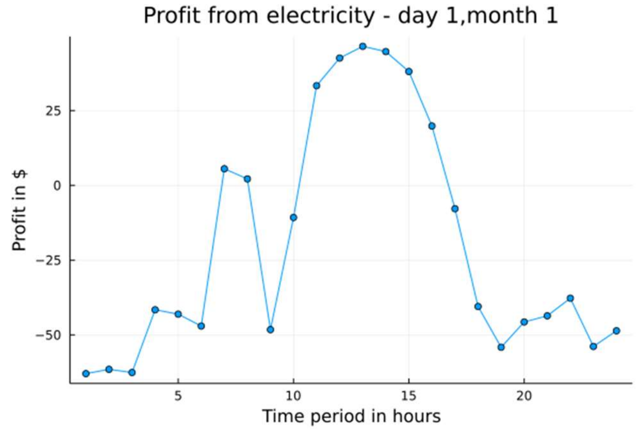

Figure 10 – Profit from electricity

As an illustrative example, several hourly decisions and parameters of day 1 month 1 are shown in Figures 6-10. The effect of the mode switching can be seen from the result. An example is illustrated above in Figure 7 where all the blue dots represent the mode at each hour. When the electricity price is low, the STC mode is preferred, when the price is moderately high the ODC mode is preferred and when the price is extremely high the shutdown mode is preferred. This is because the STC mode consumes high power but does not consume any oxygen, while the ODC mode consumes relatively lower power and consumes oxygen. Thus, these two competing effects (consumption of oxygen and power) choose the mode appropriately for each hour.

Figure 9 is a plot of the power consumed and power produced by the entire system for representative day 1 of month 1. Figure 10 shows the profit from electricity for representative day 1 of month 1. Power is sold or bought from the utility grid depending on the net effect of the power consumed by the plant, the power generated by the solar panels and wind turbines, and the power loss through the transmission lines.

These trends apply for each hour. What can be seen from Figure 6 is that there is a peak in the electricity price in hour 7. The power produced in hour 7 is negligible and thus electricity must be taken from the grid if required. To make the model profitable, the plant runs in Shut down mode as seen in Figure 7 and the profit is close to 0 as seen in Figure 10. Thus, when the electricity price is at its highest and the power produced is relatively small, the plant chooses the Shutdown mode and the profit from electricity is negligible.

Another interesting observation is in hour 13 when the profit from electricity is at its peak for the day. The electricity price is at a moderate price and hence the ODC mode is chosen. The power produced is the second highest of the day as seen in Figure 9, The peak for the power produced occurs at hour 14, where the electricity price is lower than that of hour 13 and this price makes the profit in hour 14 lower as compared to the profit in hour 13.

Conclusions

Electrification is a solution being explored to tackle the problem of greenhouse gas emissions by the chemical industry. Electrification using renewable sources of energy includes spatial and temporal variations which can affect plant production. An MILP model is proposed to deduce the optimum configuration of a network of modular plants, power generating units, and transmission lines connected by a microgrid considering spatial and temporal variations in electricity price as well as weather conditions. The model takes decisions in three-time scales: one-time investment decisions, monthly decisions like transportation as well as hourly operating decisions. A bi-level decomposition method is proposed to obtain a near-optimal solution efficiently.

The model is tested on a case study with 5 candidate locations in Western Texas with data obtained from various sources. The mode of the plant is chosen depending on the power produced and the electricity price. The power produced, power consumed/lost, and electricity price decides the profit. The major contributor to the profit is found to be the materials (products and raw materials). Electricity is found to have a significant contribution and thus the spatial location can affect the profit. The mode switching and the profit from electricity are found to be consistent with the theoretical trends. In the future, we would like to test the model on a larger dataset (more candidate locations) and test the bi-level decomposition algorithm on these cases to evaluate its computational performance.

References

Ahlhaus, P., & Stursberg, P. (2013). Transmission capacity expansion: An improved Transport Model. *IEEE PES ISGT Europe 2013*, 1–5. https://doi.org/10.1109/ISGTEurope.2013.6695322

Allman, A., & Daoutidis, P. (2018). Optimal scheduling for wind-powered ammonia generation: Effects of key design parameters. *Chemical Engineering Research and Design*, *131*, 5–15. https://doi.org/10.1016/J.CHERD.2017.10.010

Brée, L. C., Perrey, K., Bulan, A., & Mitsos, A. (2019). Demand side management and operational mode switching in chlorine production. *AIChE Journal*, *65*(7), e16352. https://doi.org/https://doi.org/10.1002/aic.16352

Deforest, N., Cardoso, G., Brouhard, T., & USDOE. (2018). *Distributed Energy Resources Customer Adoption Model (DER-CAM) v5.9*. https://doi.org/10.11578/dc.20181016.2

Cooper, N., Horend, C., Röben, F., Bardow, A., & Shah, N. (2022). A framework for the design & operation of a large-scale wind-powered hydrogen electrolyzer hub. *International Journal of Hydrogen Energy*, *47*(14), 8671–8686. https://doi.org/10.1016/J.IJHYDENE.2021.12.225

Demirhan, C. D., Tso, W. W., Powell, J. B., & Pistikopoulos, E. N. (2019). Sustainable ammonia production through process synthesis and global optimization. *AIChE Journal*, *65*(7), e16498. https://doi.org/https://doi.org/10.1002/aic.16498

ERCOT: Real-time price - LCG consulting. (n.d.). In *EnergyOnline*. http://www.energyonline.com/Data/GenericData.aspx?DataId=4

Guerra, O. J., Eichman, J., Kurtz, J., & Hodge, B. M. (2019). Cost Competitiveness of Electrolytic Hydrogen. *Joule*, *3*(10), 2425–2443. https://doi.org/10.1016/J.JOULE.2019.07.006

He, G., Mallapragada, D. S., Bose, A., Heuberger, C. F., & Gençer, E. (2021). Hydrogen Supply Chain Planning With Flexible Transmission and Storage Scheduling. *IEEE Transactions on Sustainable Energy*, *12*(3), 1730–1740. https://doi.org/10.1109/TSTE.2021.3064015

Kelley, M. T., Do, T. T., & Baldea, M. (2022). Evaluating the demand response potential of ammonia plants. *AIChE Journal*, *68*(3), e17552. https://doi.org/https://doi.org/10.1002/aic.17552

Lara, C. L., & Grossmann, I. E. (2016). Global Optimization for a Continuous Location-Allocation Model for Centralized and Distributed Manufacturing. *Computer Aided Chemical Engineering*, *38*, 1009–1014. https://doi.org/10.1016/B978-0-444-63428-3.50173-9

Mahmoud, M. S., Azher Hussain, S., & Abido, M. A. (2014). Modeling and control of microgrid: An overview. *Journal of the Franklin Institute*, *351*(5), 2822–2859. https://doi.org/10.1016/J.JFRANKLIN.2014.01.016

Ochoa Bique, A., & Zondervan, E. (2018). An outlook towards hydrogen supply chain networks in 2050 — Design of novel fuel infrastructures in Germany. *Chemical Engineering Research and Design*, *134*, 90–103. https://doi.org/10.1016/J.CHERD.2018.03.037

Palys, M. J., Allman, A., & Daoutidis, P. (2019). Exploring the Benefits of Modular Renewable-Powered Ammonia Production: A Supply Chain Optimization Study. *Industrial & Engineering Chemistry Research*, *58*(15), 5898–5908. https://doi.org/10.1021/acs.iecr.8b04189

Sampat, A. M., Kumar, R., Pushpangatha Kurup, R., Chiu, K., Saucedo, V. M., & Zavala, V. M. (2021). Multisite supply planning for drug products under uncertainty. *AIChE Journal*, *67*(1), e17069. https://doi.org/https://doi.org/10.1002/aic.17069

Tickner, J., Geiser, K., & Baima, S. (2021). Transitioning the Chemical Industry: The Case for Addressing the Climate, Toxics, and Plastics Crises. *Environment: Science and Policy for Sustainable Development*, *63*(6), 4–15. https://doi.org/10.1080/00139157.2021.1979857

Wang, H., Daoutidis, P., & Zhang, Q. (2021). Harnessing the Wind Power of the Ocean with Green Offshore Ammonia. *ACS Sustainable Chemistry & Engineering*, *9*(43), 14605–14617. https://doi.org/10.1021/acssuschemeng.1c06030

Welder, L., Ryberg, D. S., Kotzur, L., Grube, T., Robinius, M., & Stolten, D. (2018). Spatio-temporal optimization of a future energy system for power-to-hydrogen applications in Germany. *Energy*, *158*, 1130–1149. https://doi.org/10.1016/J.ENERGY.2018.05.059