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Geospatial Network Approach for Assessing Economic Potential of Ethylene-to-Fuel Technology in the Marcellus Shale Region

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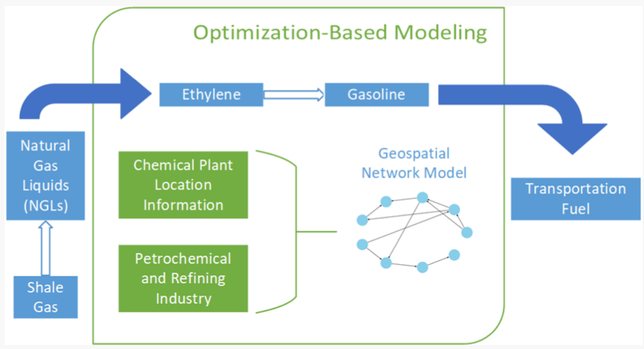
ABSTRACT: The Marcellus Shale region is rich in natural gas liquids (NGLs) and a likely future hub for NGL derivatives such as ethylene. A geospatial network model of the U.S. petrochemicals and refining industry is developed and utilized to assess the potential for the adoption of a technology for oligomerization of ethylene to gasoline, or a gasoline blend stock, as a means to utilize NGL derivatives available in the region. The model is a mixed-integer linear program with the objective of minimizing the total annual cost incurred by the regional industry. Case studies in which this technology is added to the industry network model are described, and sensitivity analyses are conducted to investigate the effect of model parameters such as the prices of crude oil and ethylene. These results can be used as cost target benchmarks for this new technology. More broadly, this work demonstrates a geospatial network modeling approach for evaluating new processing technology.



1. INTRODUCTION

The United States transitioned from being an energy importer to being an energy exporter in 2019 for the first time since the 1950s.[1] This is mainly because new technologies, such as horizontal drilling and hydraulic fracturing, have emerged and enabled hydrocarbon production, including natural gas liquids (NGLs), from the country's shale resources.[2,3] NGLs comprise predominantly ethane, propane, butane, and isobutane, with smaller amounts of pentane and less volatile hydrocarbons. NGLs are most frequently used as feedstocks for chemicals and fuel production.[4,5] The recent availability of abundant and low-cost NGLs has driven investments in chemical manufacturing, in the form of new plants, expansions of existing plants, improvements in technologies, as well as the development of new technologies.[2,6,7] For example, new ethylene manufacturing operations relying on NGL feedstocks were built or are being built in Pennsylvania,[7] Texas,[8] and Louisiana.[9]

While ethylene is a key petrochemical feedstock for producing polyethylene, ethylene glycol, styrene, and many other derivatives, the unprecedented growth in ethylene production, driven by the availability of abundant and low-cost NGLs, has led to concerns about its overproduction and the presence of excess capacity.[10] A potential high volume use for ethylene is the production of liquid transportation fuels, such as jet fuel[11] and gasoline.[5] Our focus in this work is on the oligomerization of ethylene to gasoline or a gasoline blend stock. Gasoline consumption was about 8.03 million barrels (337 million gallons) per day in the United States alone in 2020[12] and refining capacity is often tight, having grown only very slowly in recent years. Thus, an ethylene to gasoline pathway may be desirable and economically interesting.[10,13]

The economics underlying the introduction of a new technology such as ethylene to gasoline are complex and involve many considerations, including production location(s) and capacities, available transportation infrastructure, and competition with existing technologies. All of these factors must be considered to assess the potential for success of this use of ethylene and to identify its impact on the supply chains for ethylene and its derivatives. Motivated by this, we have developed a spatially resolved network model of the refining and chemical manufacturing industry to investigate the potential adoption and impact of an ethylene to gasoline technology. Based on the model formulated by DeRosa et al.,[14] the spatially resolved network model is a mixed-integer linear program that aims to minimize total industry production costs and transportation costs. We use the model to address the following key questions:

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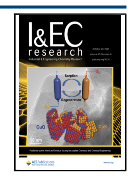

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- What is the net production cost threshold for market penetration of an ethylene to gasoline oligomerization process in the Marcellus shale region? That is, what is the *maximum adoption cost*—the largest net production cost value at which this technology will be adopted into the industry network?
- What is the extent of adoption of the new technology at net production costs below the maximum adoption cost? That is, what oligomerization capacity should be built and how does this change as the net production cost is varied?
- How does the adoption of ethylene oligomerization technology affect total industry cost and impact other parts of the refining and chemicals manufacturing industry?
- What is the optimal location for new oligomerization process units?

Since there are other, perhaps unknown, factors that also may influence the viability of the new technology, we will also perform sensitivity analyses on key model parameters. Specifically, we probe:

- What is the effect of the yield to gasoline in the oligomerization process?
- What is the impact of changes in raw material costs (crude oil and ethylene) for the competing gasoline production routes?
- What is the impact of oligomerization plant capacity?

From a broader perspective, the key objectives and contributions of this work are:

- To demonstrate, through the specific scenarios, case studies, and analyses presented, a general geospatial network modeling approach for evaluating new processing technology and assessing its impact on chemical manufacturing and refining industry networks,
- To illustrate a high-level approach for setting cost targets for technology research, development, and commercialization in the hydrocarbon processing industry

The paper first provides background on industry network models, and a description of the model formulation. Then, case studies and results are presented and discussed.

2. BACKGROUND

The refining and chemical manufacturing industry is a complex network of interconnected processes that convert basic raw materials to final products. Products or byproducts from a given process may be used as intermediates (raw materials for other processes) or become final products. There are often multiple pathways, involving different feedstocks and chemical transformations, for the production of a given material.

To represent relationships between raw materials, production technologies, and final products, a network model is utilized. Network models are database models used to represent objects and their relationships. Mathematically, a network model is often represented as a directed graph, where objects are nodes and relationships are edges (inputs and outputs) connecting the nodes. Optimization-based, input–output representations of the petrochemical industry were pioneered by Stadtherr and Rudd,[15−18] who developed linear programming (LP) models with the objective of determining the configuration of the industry that minimizes raw material consumption (amount of feedstock carbon). A multiperiod version of the model[16] based on this objective was utilized to study the evolution of the industry over three decades. This approach was also used to study the impact of adding new technologies to the industry network[17] and the impact of switching to different raw materials,[18] e.g., from fossil-based to renewable bio-based feedstock. In all of these applications, the industry network was treated as a superstructure that included not only currently used technology but other commercially proven processes that could potentially be adopted in the optimal network configuration.

Since these initial efforts, there have been several extensions and new applications of network modeling for the hydrocarbon processing industry. Sophos et al.[19] developed a model using energy-based objective functions. In this case, three different objectives were considered: maximization of thermodynamic availability change, minimization of lost work, and minimization of resource consumption. The three different cases were solved individually to obtain the optimal industry configuration for each case and then as a multiobjective program. Rudd et al.[20] developed a cost-based model that was then used by Fathi-Afshar et al.[21] to study the introduction of new technologies into the existing network. It was also demonstrated[22] how this model could be used for long-term industry planning and to study[23] the impact of restrictions on the use of toxic substances. To further study this last issue, Fathi-Afshar and Yang[24] developed a multiobjective model to seek compromise solutions using both cost- and toxicity-based objectives. The multiobjective approach was also used by Sokić et al.,[25] who focused on the impact of using alternative raw materials, and by Chang and Allen,[26] who combined a minimum-cost-based objective with minimization of chlorine use. A regional model focusing on sustainability was formulated by Al-Sharrah et al.,[27] with application to the development of the petrochemical industry in Kuwait. Here, multiple processes were available for producing a given material, and it was desired to choose only one of the alternatives, thus leading to a mixed-integer linear programming (MILP) model. The accelerated development of Kuwait's petrochemical industry shares some similarities with the current changes in the U.S. industry due to the increased shale-based hydrocarbon resources. More recently, DeRosa and Allen[28−30] formulated a next-generation industry network model based on current industrial stoichiometry derived from the IHS 2012 Process Economic Program Yearbook.[31] This was used to study the impact of raw material price changes in the supply chain, as well as to perform a case study on the potential adoption of a methane-to-aromatics process. This model was also used[32] in connection with sustainability metrics to perform consequential life cycle analysis (LCA). In the consequential approach to LCA (as opposed to the attributional approach), the indirect consequences of using a product or process are captured together with the direct effects. A similar model-based method for consequential LCA has also been given by Calvo-Serrano and Guillén-Gosálbez.[33] While our focus is on a particular industry sector and region, the use of input–output network models (Leontief models[34]), with or without an optimization component, is widespread and extends both to much larger systems (e.g., the economies of entire countries[35−37]) and to much smaller systems (e.g., the unit operation network of a specific process, such as ethylene manufacture[38,39]).

The superstructure-type models discussed above do not typically account for the specific geographic locations of the

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industrial processes used (other than to place them in a specific country or region) or the industry costs that are not directly correlated with production (e.g., transportation costs). However, there has been much work[40−43] conducted on models that do account for such cost and location data, not only for the refining and chemical manufacturing industry (or parts of it) but for other industrial sectors as well. The work of Elia et al.[44] and DeRosa et al.[14] is particularly relevant. Elia et al.[44] developed an MILP supply-chain optimization framework for natural gas to liquid (GTL) transportation fuels in the United States, with the goal of choosing optimal locations for additional GTL sites while minimizing the industry cost. This model is quite detailed and incorporates production and transportation costs on national, regional, or statewide scales. DeRosa et al.[14] developed a geospatially resolved LP model of the entire U.S. refining and petrochemical industry, based on the 2017 ICIS Supply and Demand Database,[45] to study the impacts on the industry of disruptions caused by Hurricane Harvey. In this case, a cost-based objective function was not used, the goal instead being to maximize production in the face of disruptions. Our present work is based on a geospatially resolved model formulation;[14] however, it is modified to include production and transportation costs and adapted for regional (rather than country-wide) analyses. This new model will allow us to address the key questions and sensitivity analyses identified above.

3. MODEL DESCRIPTION

3.1. Overview and Assumptions. The model was formulated as a directed graph with nodes representing existing chemical manufacturing units and potential new units, as well as material sources and sinks, with each node characterized by geographic coordinates. The graph edges represent material flows from supply nodes to new or existing chemical manufacturing units and then on to other manufacturing units or sinks. Figure 1 shows the directed graph for a very small example system, with three manufacturing unit nodes, four supply nodes, and two sink nodes. This modeling framework is general and could be used to model the entire United States or any region of the country. However, a region in the Northeastern/Eastern part of the United States was chosen because of its proximity to the Marcellus and Utica oil and gas production regions. This area of focus includes the states of North Carolina, South Carolina, Kentucky, Virginia, West Virginia, Ohio, Massachusetts, Delaware, Connecticut, Maine, Vermont, Maryland, New Hampshire, New Jersey, Pennsylvania, Rhode Island, and New York, as shown by the blue shaded area in Figure 2.

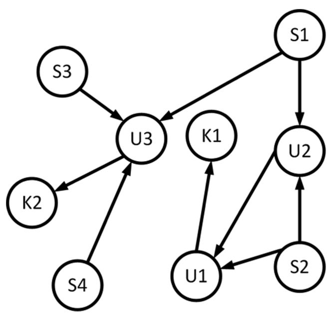

Figure 1. Directed graph for the small example system with four supply nodes, three unit nodes, and two sink nodes; "S" denotes supply nodes, "U" manufacturing unit nodes, and "K" sink nodes.

Following DeRosa et al.,[14] the locations of existing manufacturing processes in the United States, as well as the main product and capacity of each plant, were obtained from the 2017 ICIS Supply and Demand Database.[45] Data on the manufacturing process costs (adjusted for inflation[46]) and the stoichiometries of the technologies used were obtained from the IHS 2012 Process Economic Program Yearbook.[31] Manufacturing processes within the specified region were treated as manufacturing unit nodes in the model. Manufacturing processes outside the specified region were treated in the model as supply nodes capable of providing feedstocks to the unit nodes within the region. Import supply nodes and export sink nodes were placed at the Newark Port, one of the largest in the United States. For the case studies considered here, this means that this port is assumed to be a future site for ethylene export, and that a small export demand is imposed. Supplies of some materials, mostly auxiliary materials used in small quantities by a single process, were treated as exogenous (i.e., coming from outside the model network). These nodes were not assigned a specific geographic location; instead, the distance to these supplies (needed to compute transportation costs) was treated as fixed and equal to the maximum plant-to-plant distance in the area of interest. Sink nodes represent exogenous product demand (i.e., use outside the network) and, except for export sink nodes, were not assigned a location (it was assumed that products are sold free on board (FOB) at the production point or export node, so the exogenous purchaser pays the transportation cost from that point). A special ethylene supply node was placed in Pennsylvania at the site of the Shell Chemical Appalachia LLC ethane cracking facility that is expected to begin production in the early 2020s using ethane from the Marcellus Shale[7] to supply ethylene for colocated polyethylene production. Consistent with the scenario of overcapacity for ethylene and polyethylene, it was assumed that there is no polyethylene production at this location and that all of the ethylene capacity here can be used to supply potential oligomerization gasoline units or for export and the production of other derivatives.

A map showing the locations of unit nodes and supply nodes in the model, as well as relative capacities, is shown in Figure 2. The goal in applying the model is to assess the potential adoption of an oligomerization of ethylene to gasoline process in the Marcellus-Utica region. These potential manufacturing units were placed in locations that already have existing manufacturing units to take advantage of the existing infrastructure. Ultimately, the model will be used to determine which of these potential plant locations are optimal.

3.2. Technology of Interest. Ethylene oligomerization can be operated to generate an array of products. For example, Toch et al.[49,50] show that, by choice of operating conditions and catalyst design, one can produce a predominantly linear α-olefin product or a predominantly C_{5+} branched gasoline product. The Siluria process[13] for producing gasoline from ethylene is claimed to have extremely high ethylene conversion and product selectivity. Furthermore, Toch et al.[50] indicate that a 99% conversion (based on ethylene consumption) and a 50% selectivity toward a gasoline product could be achieved, with selectivity defined on a carbon basis as

$$S_i = \frac{a_{C,i}}{2} \frac{F_i}{F_{C_2}^{\circ} - F_{C_2}} \tag{1}$$

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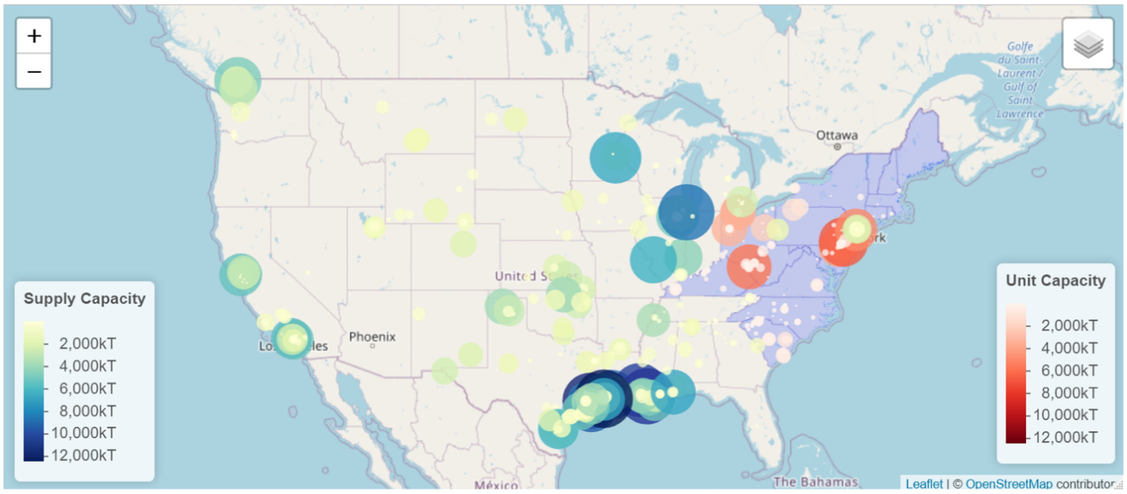

Figure 2. Map showing the locations of manufacturing units and supply units in the model. Manufacturing units are shown in the shades of red and supply units are shown in the shades of green and blue. The shaded area shows the states that are included in the region of interest. Figure is created by leafletR[47] using map tiles from OpenStreetMap.[48]

Here, S_i is the selectivity to product i, $a_{C,i}$ is the number of carbon atoms of product i, F_i is the molar flow rate of product i, $F^{\circ}_{C_2}$ is the ethylene molar feed rate, and F_{C_2} is the ethylene molar outlet flow rate. Assuming that the ratio of product carbon number to ethylene carbon number $(a_{C,i}/2)$ is approximately the same as the ratio of product molecular weight to ethylene molecular weight (M_i/M_{C_2}), then selectivity based on carbon number will be approximately equal to selectivity based on mass. Thus, as a base case for this technology, we have assumed that the consumption of ethylene for the production of 1 kg of gasoline is 2 kg. At these conditions (99% ethylene conversion, 50% selectivity to gasoline), Toch et al.[50] find that there is also 25% selectivity to propylene with the remaining carbon in a C_4 fraction (butenes). The propylene byproduct can itself be oligomerized to gasoline,[51] which can significantly increase the overall gasoline yield, and depending on the composition of the C_4 fraction, it may also contribute to the gasoline yield or provide other useful byproducts. Since the ultimate yield to gasoline can vary, we will present studies below that consider the sensitivity of results to this parameter.

In the base case with 50% yield to gasoline, it will be assumed that the mixed byproducts can be used as fuel by colocated chemical manufacturing facilities. Assuming a net heating value of about 19550 BTU/lb (based on 50% propylene, 50% butenes), and a price of \$2/MMBTU, a byproduct credit for 50% yield of gasoline of \$86/t of gasoline produced was assumed.

3.3. Model Formulation.

As noted above, the industry network model is a modification of the directed graph model of DeRosa et al.[14] The formulation of this model, as modified, is summarized here. The set of all nodes is denoted as N. The set of supply nodes is denoted by S, the set of existing chemical manufacturing unit nodes by U, the set of sink nodes by K, and the set of potential plant nodes by Z. Thus, $N = S \cup U \cup K \cup Z$. I is the set of all materials in the model. J is the set of all technologies used in the manufacturing nodes. Associated with each node $m \in U \cup K \cup Z$ is a set of input materials $I_{\text{in},m}$, and associated with each node $n \in U \cup S \cup Z$ is a set of output materials $I_{\text{out},n}$. If there is a potential material flow from node $n \in N$ to node $m \in N$, then there is a directed edge (n,m) in the graph. The set of all edges representing potential flows of material $i \in I$ is then given by $E_i = \{(n,m) \mid i \in I_{\text{out},n} \cap I_{\text{in},m}\}$.

The model is a mixed-integer linear program (MILP) with the objective to minimize the industry's total annual cost

$$C_{\text{tot}} = \sum_{n\in(U\cup Z)} C_{\text{p},n}P_n + \sum_{i\in I}\sum_{\substack{(n,m)\in E_i\\ m\notin K}} C_{\text{t}}Y_{i,n,m}d_{n,m} \quad (2)$$

where C_{tot} is the total annual industry cost, $C_{\text{p},n}$ is the net cost of production (per unit mass of main product) for node n, P_n is the production level (mass flow rate of main product) for node n, C_{t} is an average cost for transportation, $d_{n,m}$ is the distance (straight line) between nodes n and m, and $Y_{i,n,m}$ is the magnitude of the mass flow rate of material i from node n to node m. The first term in eq 2 accounts for the net production cost incurred at the existing and potential manufacturing unit nodes. The net production cost coefficients $C_{\text{p},n}$ include raw material costs (less byproduct credits), capital cost recovery, utility costs, and other operating costs (e.g., maintenance, labor, overhead, taxes). The second term in eq 2 accounts for transportation costs between nodes. The current model includes transportation costs from supply nodes to manufacturing nodes, from one manufacturing node to another manufacturing node, and from manufacturing nodes to export nodes. Transportation costs from manufacturing nodes to sinks (other than export nodes) are not accounted for, as it is assumed that final products are sold FOB at the production point or export node. The model does not distinguish between different transportation modes used in the industry (rail, truck, pipeline, ship). The unit transportation cost (per metric ton per mile) is assigned a value of C_{t} = \$0.1883/t·mi based on transportation by truck.[52] This will place a relatively strong weight on transportation cost and accordingly influence the choice of location for new facilities.

As mentioned earlier, the potential unit manufacturing nodes (ethylene to gasoline) are placed in locations with existing chemical plants to take advantage of existing infrastructure (multiple nodes, each representing a different technology, can exist at the same geographic location). It is assumed that each potential new plant will be at a different location. Binary variables $\beta_n \in \{0, 1\}$, $n \in Z$ are introduced to represent each of these potential units. In the optimization problem, the number and location of the potential plants chosen for production will be determined. Potential nodes selected for production will have $\beta_n = 1$ and those not selected will have $\beta_n = 0$. If a node $n \in Z$ is selected, it is assumed that it will operate at full capacity C_n, so that the production level of the potential plants is $P_n = \beta_n C_n$, $\forall n \in Z$. A base case new plant capacity of 200 KTA (thousand metric tons per year) was chosen because it is comparable to conventional GTL plant capacities.[53] However, the effect of changing the plant size will be considered.

It is assumed that there is a limit on the investment capital available to build new manufacturing units. However, there is limited information to carry on a detailed capital cost estimate for the ethylene oligomerization process. Thus, we will impose a capital cost constraint indirectly, by first assuming that the capital cost for different plant capacities is given by

$$C_{c,n} = C_{c,200}\left(\frac{C_n}{200}\right)^{0.8}\beta_n, \quad \forall n \in Z \tag{3}$$

where $C_{c,n}$ is the capital cost for a unit of capacity C_n (in KTA) and $C_{c,200}$ is the capital cost required for a 200 KTA plant. The scaling coefficient of 0.8 is based on capital cost data[31] for a similar gas to liquids process. The total capital cost for new units is then subject to an upper limit to account for practical financial limitations

$$\sum_{n \in Z} C_{c,n} = \sum_{n \in Z} C_{c,200}\left(\frac{C_n}{200}\right)^{0.8}\beta_n \le C_{c,tot} \tag{4}$$

where $C_{c,tot}$ is the total investment capital available. The available capital is then set so that no more than five 200 KTA units can be built

$$C_{c,tot} = 5C_{c,200} \tag{5}$$

This gives the final indirect capital cost constraint of

$$\sum_{n \in Z}\left(\frac{C_n}{200}\right)^{0.8}\beta_n \le 5 \tag{6}$$

This capital constraint is imposed to manage investment risk. We are considering a new technology adoption, and it is unreasonable to assume that there will be immediate large-scale implementation. By allowing, however, a small number of plants to be adopted, we are able to study the industry effects from these adoptions.

The material balance constraints in the model for each type of node are now described:

1. Supply nodes: a supply node $n \in S$ for material i takes a supply stream $P_n = X_{i,n}$ and divides it into separate streams that will supply the unit nodes with material i

$$\sum_{m \in U} Y_{i,n,m} = X_{i,n}, \quad \forall n \in S \tag{7}$$

2. Unit and potential plant nodes: in each of these nodes $n \in U \cup Z$, required materials $i \in I_{in,n}$ are first collected from supply nodes and other unit and potential plant nodes and then combined into raw material streams $X_{i,n}$

$$\sum_{m \in (U \cup S \cup Z)} Y_{i,n,m} = X_{i,n}, \quad \forall i \in I_{in,n}, \forall n \in (U \cup Z) \tag{8}$$

The raw material streams then undergo transformation into product streams using technology $j_n \in J$ according to a specified stoichiometry

$$X_{i,n} = a_{i,j_n} X_{b_{j_n},n}, \quad \forall i \in I_{in,n} \cup I_{out,n}, \forall n \in (U \cup Z) \tag{9}$$

where a_{i,j_n} is the input−output coefficient of material i in technology j_n relative to the main product (basis species) $b_{j_n} \in I$ and $X_{b_{j_n},n} = P_n$ is the main product flow. Finally, for each produced material $i \in I_{out,n}$, the produced stream $X_{i,n}$ is divided and distributed to other unit, potential plant, or sink nodes

$$X_{i,n} = \sum_{m \in (U \cup K \cup Z)} Y_{i,n,m}, \quad \forall i \in I_{out,n}, \forall n \in (U \cup Z) \tag{10}$$

3. Sink nodes: a sink node $n \in K$ for material i collects produced i from the unit and potential plant nodes and determines a produced amount $P_n = X_{i,n}$

$$X_{i,n} = \sum_{m \in (U \cup Z)} Y_{i,m,n}, \quad \forall n \in K \tag{11}$$

In addition to constraints imposed by eqs 6−11, there are constraints on supply, demand, and unit capacity, as well as nonnegativity of flows. The demand constraint on the sink nodes requires that the produced amount P_n for node $n \in K$ at least satisfy a specified demand D_n

$$P_n = X_{i,n} \ge D_n, \quad \forall n \in K \tag{12}$$

The supply constraint on supply nodes requires that the supplied amount P_n for node $n \in S$ not exceed a specified supply capacity C_n

$$P_n = X_{i,n} \le C_n, \quad \forall n \in S \tag{13}$$

The capacity constraint on manufacturing unit nodes requires that the production of the main product in an existing unit node $n \in U$ not exceed a specified unit capacity C_n

$$P_n = X_{b_{j_n},n} \le C_n, \quad \forall n \in U \tag{14}$$

and, as discussed above, for a new manufacturing node $n \in Z$, the capacity constraint is

$$P_n = \beta_n C_n, \quad \forall n \in Z \tag{15}$$

Nonnegativity of flows requires

$$X_{i,n} \ge 0, \quad \forall n \in N, \forall i \in (I_{in,n} \cup I_{out,n}) \tag{16}$$

and

$$Y_{i,n,m} \ge 0, \quad \forall i \in I, \forall (n, m) \in E_i \tag{17}$$

The final MILP minimization problem now consists of the objective function given by eq 2 and constraints given by eqs 6−17. Decision variables in the MILP are those appearing in nonnegativity constraints, eqs 16 and 17 and binary variables β_n, $n \in Z$. The number of decision variables can be reduced by algebraic elimination using the constraints; however, for clarity in describing the model formulation, we have not done this here. This MILP model was implemented using the General Algebraic Modeling System (GAMS).[54]

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3.4. Model Limitations. Even though different transportation modes (rail, pipeline, ship, truck) are used in the chemical industry, the model does not distinguish between different modes. Instead, the transportation cost component is based on an average cost associated with truck transportation. Due to limited information, the capital cost of new manufacturing units (ethylene to gasoline) is not explicitly estimated. Annualized capital cost recovery is assumed to be included in the net production cost, and a cap on the number of new units is imposed to limit investment risk. The stoichiometries and operating costs used in the model are taken from the IHS 2012 Process Economic Program Yearbook.[31] Even though this is not the most up-to-date database, process stoichiometries do not generally change significantly with time, and operating costs have been adjusted for inflation. The set of existing plant units is based on the 2017 ICIS Supply and Demand Database.[45] New plant units starting up since then or currently under construction are not accounted for, with the exception of the Shell Chemical Appalachia LLC ethane cracking facility planned to begin production in the Marcellus Shale region in the early 2020s. While we have aimed to keep the model fidelity at a high level, all industry models have multiple sources of uncertainty, the hydrocarbon processing industry especially so, due to recent price volatility in crude oil, natural gas, and ethylene prices. Sensitivity analyses will be performed to address some of this uncertainty.

4. RESULTS

4.1. Base Case. We first implement a base case study in which the maximum adoption cost, extent of adoption, and optimal plant locations for the new ethylene to gasoline process are determined for two different values of the new process unit capacity (C_n = 100 KTA and C_n = 200 KTA, $n \in Z$). As mentioned earlier, a 200 KTA capacity is comparable to conventional GTL chemical plants. The 100 KTA option is added to study the effect of plant size in technology adoption. To do this, the MILP model is solved for increasingly large values of the new process net production cost ($C_{p,n}$, $n \in Z$), in increments of \$100/t of produced gasoline, until the process no longer appears in the optimal industry (all β_n = 0). A diagram of this workflow is provided in the Supporting Information. It is assumed that the plant oligomerization yield to gasoline and overall process efficiencies are the same in both the 100 and 200 KTA cases, and that capital cost recovery is a relatively small production cost component, so that the net production cost per unit of gasoline is the same in each case. Gasoline production cost in refineries is based on a crude oil price of \$50/bbl.

4.1.1. Optimal Costs. Results for total industry costs (C_{tot}), as well as total net production costs (first term eq 2) and total transportation costs (second term eq 2), are shown in Figures 3−5, respectively. In each figure, the results for the number of oligomerization processes adopted are also overlaid. It is seen that the new ethylene oligomerization technology is adopted when its net gasoline production cost is ≤\$1000/t (net production cost after byproduct credit of \$86/t gasoline). At this cost point (the maximum adoption cost), the total annual cost becomes slightly less than the case of no adoption (this cannot be seen on the scale of Figure 3). Though the net production cost increases (since \$1000/t is greater than the cost of gasoline from refineries), the transportation cost decreases by a slightly larger amount due to less crude oil

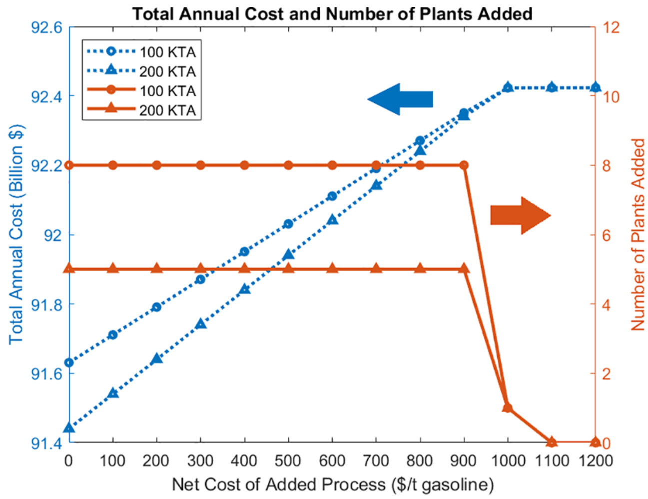

Figure 3. Comparison of region-wide optimal total annual cost and the number of plants added to the industry network for a range of process costs for both plant capacities.

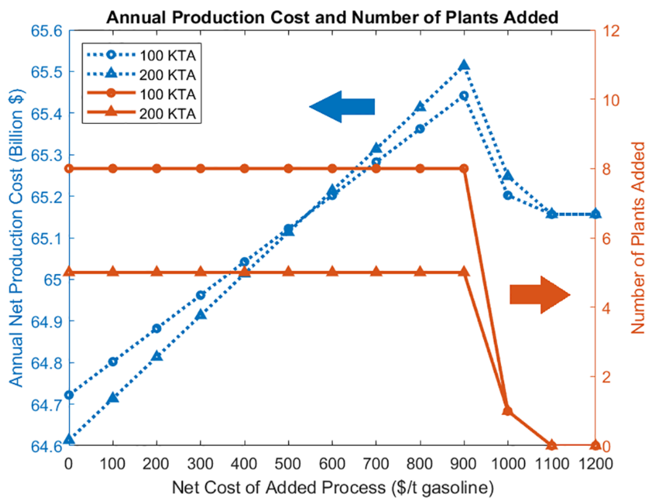

Figure 4. Comparison of region-wide optimal annual net production cost and the number of plants added to the industry network for a range of process costs for both plant capacities.

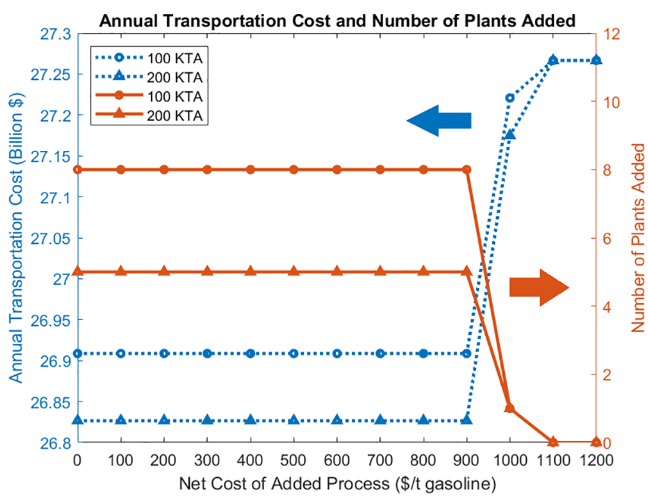

Figure 5. Comparison of region-wide optimal annual transportation cost and the number of plants added to the industry network for a range of process costs for both plant capacities.

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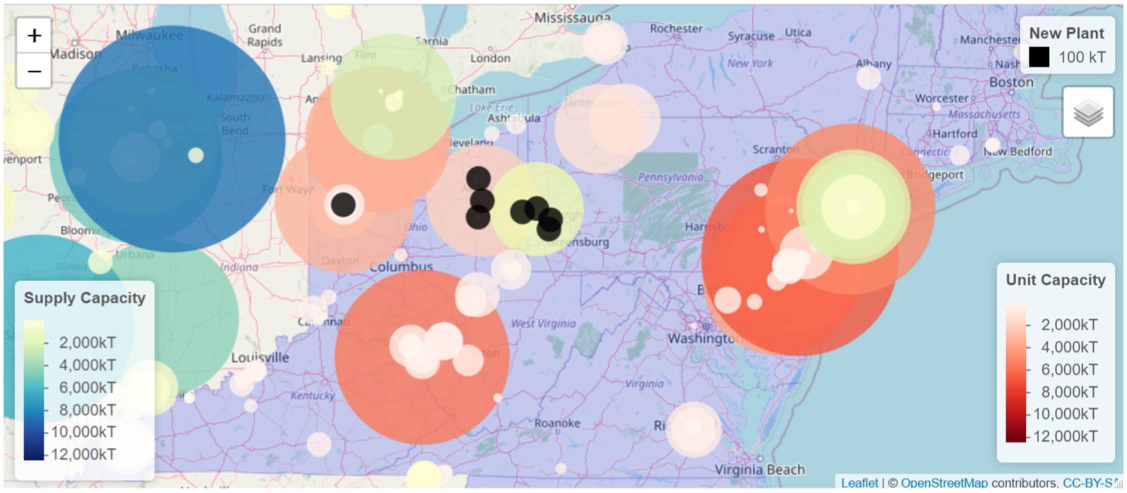

Figure 6. Location (solid black circles) of new plants for the 100 KTA case at full adoption. Other manufacturing units are shown in the shades of red and supply units are shown in the shades of green and blue. Figure is created by leafletR[47] using map tiles from OpenStreetMap.[48]

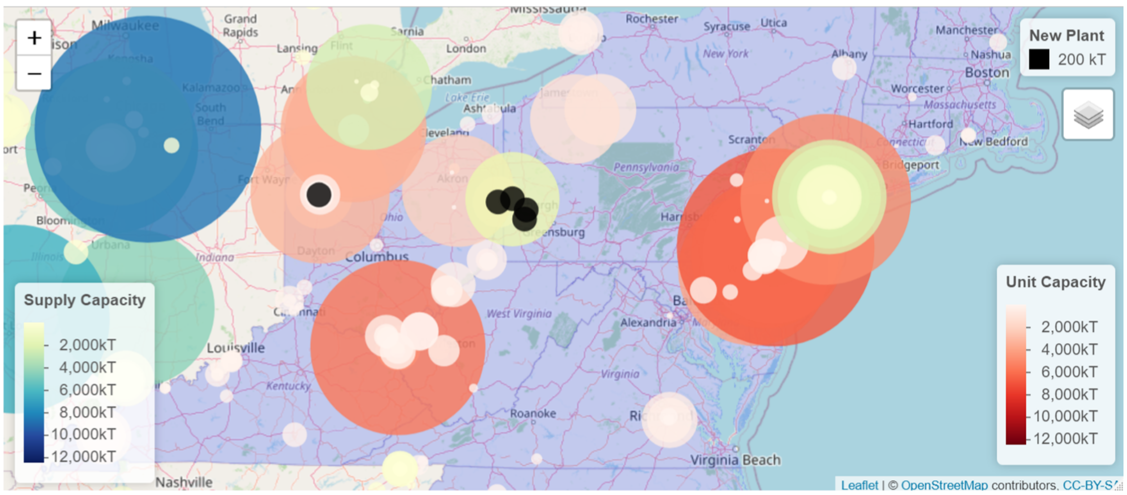

Figure 7. Location (solid black circles) of new plants for the 200 KTA case at full adoption. Other manufacturing units are shown in the shades of red and supply units are shown in the shades of green and blue. Figure is created by leafletR[47] using map tiles from OpenStreetMap.[48]

transportation to refineries (transportation cost is approximately $190/t for crude oil to refineries). At the net cost point of $900/t, full adoption has been reached for both plant sizes considered, as limited by the available capital constraint (eq 6). At full adoption, eight plants are used in the 100 KTA case (800 KTA total production) and five plants are used in the 200 KTA case (1000 KTA total production). The difference in total production between the two cases leads to the higher net production cost results (Figure 4) for the 200 KTA case at the $900/t net production cost point and the steeper total net production cost descent as the unit net production cost decreases. The crossover point (between $500/t and $600/t) between the two cases occurs at the net cost point corresponding to the net production cost of refinery-based gasoline. Total transportation costs (Figure 5) are lower in the 200 KTA case due to the smaller number of plants. This leads to results for optimal total costs (Figure 3) that favor 200 KTA capacity plants, though the 100 KTA case also leads to overall cost reduction.

4.1.2. Optimal Plant Locations. The optimal locations of the eight 100 KTA plants are shown in Figure 6. As mentioned earlier, new plants are located at sites where chemical manufacturing facilities already exist. The plants are located in three states:

- Ohio: Akron, Canton, Dover, and Lima
- Pennsylvania: Bridgeville, Monaca, and Neville Island
- West Virginia: Newell

Most of the new plants are located in the vicinity of the planned Shell Chemical Appalachia LLC ethane cracker in Pennsylvania.[7] This is expected because their location near an ethylene source node leads to lower transportation costs and because the full ethylene capacity of this cracker is assumed to be available for gasoline production. Two plants (Canton, OH and Newell, WV) also obtain some ethylene from colocated refineries. There is one plant (Lima, OH) located further away from this vicinity. This occurs because the ethylene supply capacity in the vicinity has been exhausted by the seven new plants in the area, as well as other chemical manufacturing units. Consequently, a plant is placed at Lima, OH to take advantage of colocated ethylene production, which is supplemented by some nearby ethylene byproduct from refineries in Toledo, OH. The primary impact of adding these new plants is to reduce gasoline production at a Toledo refinery, which would operate at 74% capacity when eight

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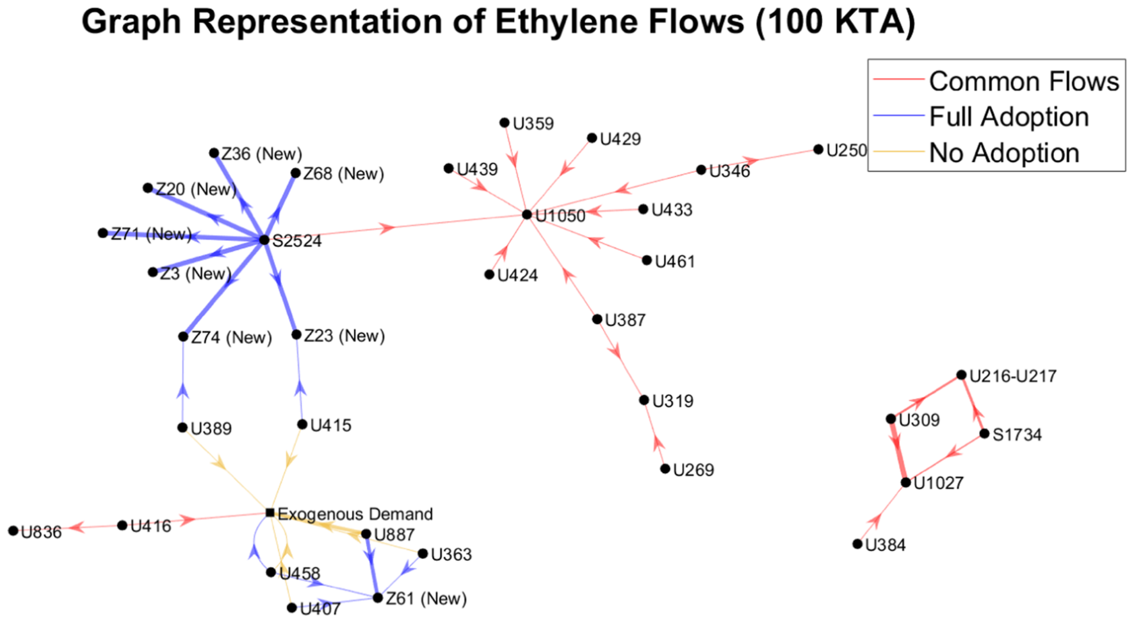

Figure 8. Graph of ethylene flows (edges), before and after full-plant adoption, between relevant nodes of the network for the 100 KTA case. Node names are identified in Tables 1 and 2.

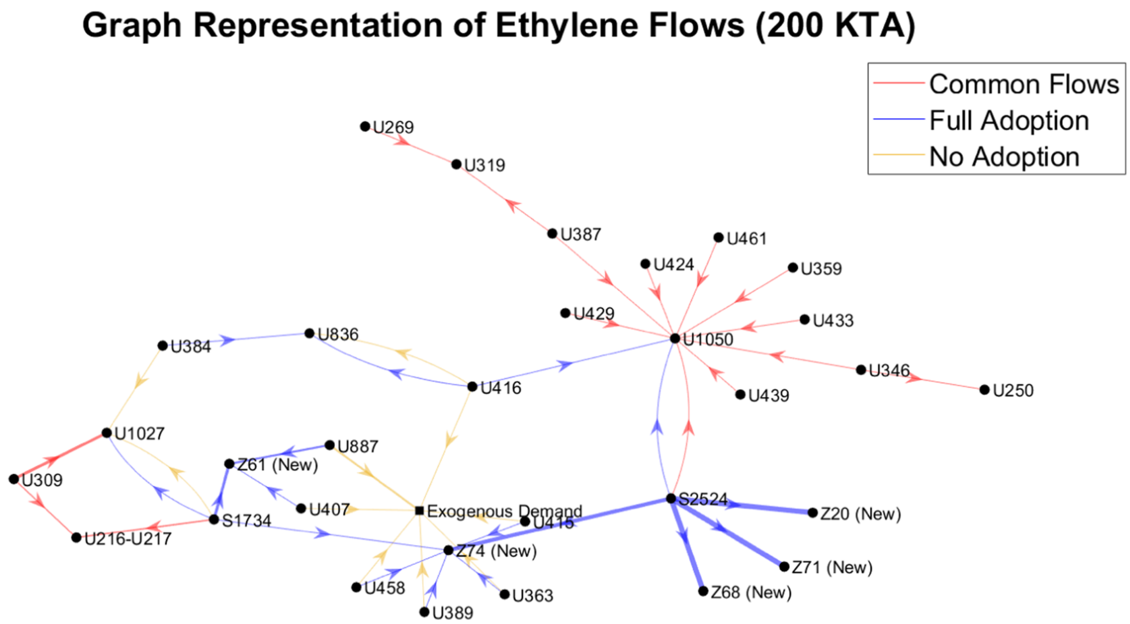

Figure 9. Graph of ethylene flows (edges), before and after full-plant adoption, between relevant nodes of the network for the 200 KTA case. Node names are identified in Tables 1 and 2.

oligomerization gasoline plants are added, and at 97% capacity when one plant is added ($1000/t net cost point). The operation of this particular refinery is reduced because of the higher transportation costs of using its products elsewhere in the network (beyond the new Lima oligomerization plant). In addition to this primary impact, there are also several secondary effects on the industry network, mostly impacting refinery coproducts and the ethylene supply chain, as discussed below.

The optimal locations of the 200 KTA plants are shown in Figure 7. Similar to the previous case, most of the new plants are located near the Shell ethane cracker, but one plant is again located further away, in Lima, OH, because of the exhaustion of the ethylene supply from the Shell cracker. The plants are located in three states:

- Ohio: Lima
- Pennsylvania: Bridgeville, Monaca, and Neville Island
- West Virginia: Newell

Again a refinery in Toledo, OH would be affected by this change, and it would operate at 68% capacity if five oligomerization gasoline plants are added and at 94% when one plant is added ($1000/t net cost point). In this case, the Lima, OH plant is supplied by colocated ethylene production and draws additional ethylene from Channahon, IL.

4.1.3. Impact on the Ethylene Supply Chain. While the direct impact of adding oligomerization gasoline plants is to

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reduce refinery gasoline production, there are also secondary effects. When a new plant is added, it is expected that flows between nodes will be altered to accommodate the "disturbance" stemming from the addition. One of the advantages of using an industry network model is that it enables the identification of such cascading impacts. In this case study, several such changes occur in the ethylene supply chain, as described in this section.

At the maximum adoption cost ($1000/t), where only one plant is added in each case (100 and 200 KTA), ethylene flows do not differ substantially from the case where there is no adoption. However, at lower net oligomerization process costs, when there is full adoption of the technology, there are significant changes in the ethylene supply chain. This is depicted schematically in Figures 8 and 9 for 100 and 200 KTA cases, respectively. The nodes appearing in these diagrams are identified in Tables 1 and 2. Numerical values for the ethylene flows are given in Table 3.

Table 1. Destinations of Ethylene Flows in Figures 8 and 9

destination node	location	material
U216-U217	Calvert City, Kentucky	ethylene dichloride
U250	Springfield, Massachusetts	ethyl acetate
U319	New Castle, Delaware	ethylene oxide
U836	Neal, West Virginia	polypropylene
U1027	Calvert City, Kentucky	vinyl chloride
U1050	Newark Port, New Jersey	ethylene (export)
Z3	Akron, Ohio	gasoline
Z20	Bridgeville, Pennsylvania	gasoline
Z23	Canton, Ohio	gasoline
Z36	Dover, Ohio	gasoline
Z61	Lima, Ohio	gasoline
Z68	Monaca, Pennsylvania	gasoline
Z71	Neville Island, Pennsylvania	gasoline
Z74	Newell, West Virginia	gasoline

Table 2. Sources of Ethylene Flows in Figures 8 and 9

source node	location	material/plant Type
S1734	Channahon, Illinois	ethylene
S2524	Potter Township, Pennsylvania	ethylene
U269	New Castle, Delaware	ethylene
U309	Calvert City, Kentucky	ethylene
U346	Bradford, Pennsylvania	refinery (ethylene byproduct)
U359	Paulsboro, New Jersey	refinery (ethylene byproduct)
U363	Toledo, Ohio	refinery (ethylene byproduct)
U384	Somerset, Kentucky	refinery (ethylene byproduct)
U387	Delaware City, Delaware	refinery (ethylene byproduct)
U389	Newell, West Virginia	refinery (ethylene byproduct)
U407	Lima, Ohio	refinery (ethylene byproduct)
U415	Canton, Ohio	refinery (ethylene byproduct)
U416	Catlettsburg, Kentucky	refinery (ethylene byproduct)
U424	Trainer, Pennsylvania	refinery (ethylene byproduct)
U429	Paulsboro, New Jersey	refinery (ethylene byproduct)
U433	Philadelphia, Pennsylvania	refinery (ethylene byproduct)
U439	Linden, New Jersey	refinery (ethylene byproduct)
U458	Toledo, Ohio	refinery (ethylene byproduct)
U461	Warren, Pennsylvania	refinery (ethylene byproduct)
U887	Lima, Ohio	ethylene

For the 100 KTA case, the main impact is that some ethylene flows to exogenous demand (use outside the current network) have been redirected to ethylene oligomerization processes. For example, refinery byproduct ethylene from the Newell, WV refinery (U389 in Figure 8) is now used in the new colocated oligomerization plant rather than used to satisfy exogenous demand. In effect, these changes transfer a disturbance in the ethylene supply chain to consumers outside the network. Since these exogenous consumers are not part of the network model, no specific destination or end use is associated with them.

Table 3. Affected Flows of Ethylene to Destination Nodes for Full Adoption of 100 KTA Plants and Full Adoption of 200 KTA Plants, with Comparison to No Adoption[a]

destination	no adoption	full adoption (100 KTA)	full adoption (200 KTA)
polypropylene (U836)	U416: 24.6	U416: 24.6	U416: 23.8
			U384: 0.8
vinyl chloride (U1027)	S1734: 58.6	S1734: 58.6	S1734: 59.4
	U384: 0.8	U384: 0.8	
ethylene export (U1050)	S2524: 12.1	S2524: 12.1	U416: 11.8
			S2524: 0.3
gasoline (Z3)		S2524: 200	
gasoline (Z20)		S2524: 200	S2524: 400
gasoline (Z23)		S2524: 186.7	
		U415: 13.3	
gasoline (Z36)		S2524: 200	
gasoline (Z61)		U887: 155	S1734: 224.1
		U407: 21	U887: 155
		U363: 14.8	U407: 20.9
		U458: 9.2	
gasoline (Z68)		S2524: 200	S2524: 400
gasoline (Z71)		S2524: 200	S2524: 400
gasoline (Z74)		S2524: 197.1	S2524: 296.6
		U389: 2.9	S1734: 51.4
			U363: 19.9
			U458: 15.9
			U415: 13.3
			U389: 2.9

[a]Ethylene source and quantities (in KTA) are shown. Node names are identified in Tables 1 and 2.

For the 200 KTA case, there are also several cases in which ethylene is diverted from exogenous demand to new oligomerization gasoline plants. However, there are also some other changes that might not have been anticipated. For example, when there are no oligomerization plants adopted, the ethylene supply for the Calvert City vinyl chloride facility (U1027 in Figure 9) comes primarily from colocated ethylene production (U309 in Figure 9), with some additional supply from Channahon (S1734 in Figure 9) and Somerset (U384 in Figure 9). However, at maximum adoption of 200 KTA oligomerization plants, the refinery in Somerset is no longer part of the supply chain for the vinyl chloride plant, and the difference is supplied by the Channahon ethylene plant. The refinery in Somerset now becomes part of the ethylene supply chain for the polypropylene plant in Neal (for random copolymer polypropylene).

4.1.4. Impact on Refinery Products. The adoption of the oligomerization technology to produce gasoline from ethylene has a direct impact on gasoline production in refineries. For the relatively small-scale adoption of oligomerization technol-

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ogy in this case study, refinery gasoline production in the region of interest is reduced by 1.9% in the 100 KTA case and 2.3% in the 200 KTA case. This may lead to similarly reduced production of refinery coproducts, such as diesel and jet fuel. However, a refinery has significant operational flexibility and may be able to direct production away from gasoline and toward these coproducts to maintain their output. Nevertheless, if the ethylene oligomerization technology were adopted on a larger scale, reduced output of refinery coproducts may still become an issue of concern. This may motivate additional technology developments for converting NGL-based feedstocks such as light alkenes into diesel and jet fuel.[11,55]

4.2. Sensitivity Analyses. The results discussed above are sensitive to changes in various model parameters, such as the prices of crude oil and ethylene, the yield to gasoline in the oligomerization process, the transportation cost coefficient C_v, and others. In this section, we focus on crude oil and ethylene prices and on the yield to gasoline; sensitivity analyses are performed to determine how changes in these quantities affect the case study results. Also, because there are alternative uses for ethylene, we consider opportunity cost in an additional sensitivity study.

4.2.1. Crude Oil Price. Crude oil prices are historically volatile and will have a direct impact on the production cost of refinery-based gasoline, which in turn will impact the maximum adoption cost for the oligomerization gasoline process. Higher oil prices will lead to the higher production cost of refinery-based gasoline, favoring adoption of the oligomerization process (allowing its adoption at higher net costs). The opposite will occur in the case of lower oil prices. Thus, a key impact of changes in the crude oil price is its effect on the maximum adoption cost for the oligomerization process. To investigate this, the case study above was repeated for a range of crude oil prices, and the maximum adoption cost for oligomerization gasoline determined. The crude oil prices considered are \$30, \$40, \$50 (base case), \$60, and \$70 per barrel.

The results for both 100 and 200 KTA plant capacities are the same, as presented in Figure 10. The plant capacity does not have an impact because of the assumptions discussed earlier concerning plant efficiencies and capital cost recovery that make the unit production cost the same for both plant capacities. The results for the maximum adoption cost clearly indicate a strong sensitivity to the crude oil price, ranging from \$600/t for oil at \$30/bbl to \$1300/t for oil at \$70/bbl. Thus, a significant drop in crude oil price could deter the adoption of an ethylene to gasoline oligomerization process, but, in the opposite case, there may be significant opportunities for the adoption of the process under consideration. However, the ethylene price is also an important consideration, as quantified in the next section.

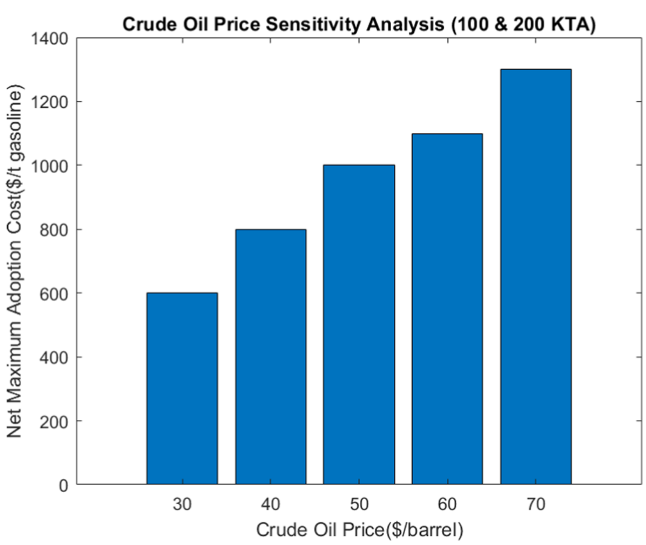

Figure 10. Maximum net adoption cost for different crude oil prices and plant capacities.

4.2.2. Gasoline Yield. The gasoline yield of the oligomerization process is clearly a key parameter. For a fixed amount of gasoline, an increase or decrease in yield will lead to a decrease or increase, respectively, in raw material (ethylene) consumption. The ethylene raw material cost is then determined both by its consumption and price. Thus, another parameter that must be considered in this context is the ethylene price. The cost of raw materials is part of the unit net production cost $C_{p,n}$ in the model; however, for purposes of this sensitivity analysis, it is convenient to split the production cost into a raw material cost, dependent on the ethylene price, and a nonmaterial cost. The byproduct credit, based on use as fuel as discussed above, is deducted from the cost of raw materials. We then will determine the range of nonmaterial production cost, as a function of yield and ethylene price, for which the oligomerization gasoline process is adopted. The sensitivity analysis will be conducted for both 100 and 200 KTA plant capacities and for 40, 50, and 60% yield to gasoline. Recent ethylene prices have fluctuated significantly.[56] To be consistent with the scenario of ethylene overproduction and excess capacity, we will use ethylene prices at the bottom of their historic price range, specifically 10, 15, and 20 cents/lb (prices seen in 2020). The price of crude oil is fixed at \$50/bbl.

The results for 200 KTA plants are shown in Figure 11. Looking first at the low yield (40%) case, for the lowest ethylene price (10 cents/lb), the maximum nonmaterial adoption cost (above which the process is not adopted) is about \$580/t of gasoline. The number of plant additions increases steeply once the nonmaterial cost goes below its maximum adoption level. At an ethylene price of 15 cents/lb, the maximum nonmaterial adoption cost is about \$300/t, and for ethylene at 20 cents/lb, it is about \$25/t. Not unexpectedly, as the yield to gasoline increases, to 50% and then 60%, adoption of the process at higher nonmaterial cost points is enabled, reaching a maximum nonmaterial adoption cost of \$690/t in the most favorable case. As in the sensitivity analysis for the crude oil price, and for the same reasons, maximum nonmaterial adoption costs are the same for 100 KTA plants and so are not shown here. However, in 100 KTA plants, the cost points at which the number of plant adoptions increases are somewhat different.

From these results, we can conclude that both the reaction yield to gasoline and the ethylene price play an important role in determining process adoption. Low ethylene prices can outweigh the negative performance of a less selective catalyst, and a more selective catalyst can provide a substantial nonmaterial cost range over which process adoption will occur, even for higher ethylene prices. Of course, one should consider that the ethylene price is volatile and controlled by supply and demand, whereas selectivity is affected by catalyst

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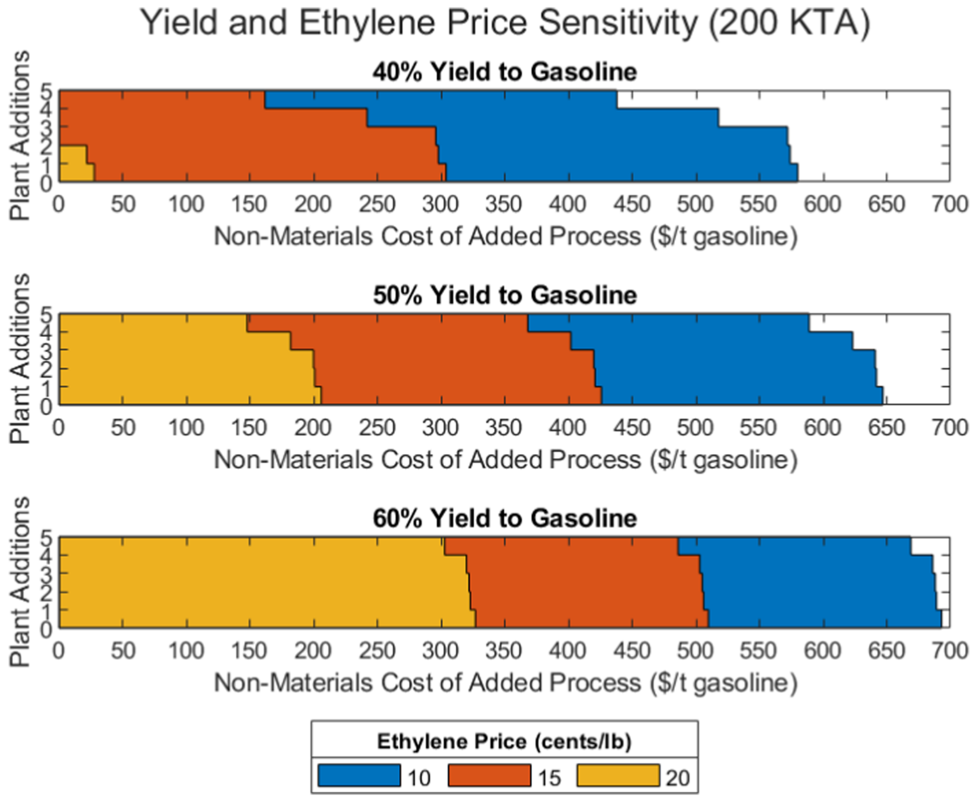

Figure 11. Range of process costs (excluding net raw material cost) for which the process is viable and the number of plant additions, for different prices of ethylene and yield to gasoline, for 200 kTA plants.

characteristics, which can potentially be improved to better suit an ethylene to gasoline oligomerization process.

4.2.3. Opportunity Cost. The decision to adopt the ethylene to gasoline technology comes with an opportunity cost since there are alternative uses for the ethylene raw material. For the region of interest, the predominant alternative use of ethylene would be for polyethylene (PE) production. A planned polyethylene facility, producing both high-density polyethylene (HDPE) and linear, low-density polyethylene (LLDPE), is colocated with the Shell Chemical Appalachia LLC ethane cracking facility in Western Pennsylvania, with both expected to come online in the early 2020s. Thus, we consider the opportunity cost of not using ethylene to produce PE.

In minimum cost processes for producing HDPE and LLDPE from ethylene, the nonethylene cost is about 16−17 cents/lb PE while using about 0.9 lb ethylene/lb LLDPE and 1 lb ethylene/lb HDPE.[31] From 2011 to mid-2015, the price margin of HDPE and LLDPE over ethylene ranged from 0 to about 27 cents/lb.[57] More recently, from May 2020 to March 2021, the price margin has ranged from about 11−26 cents/lb for HDPE and 11−21 cents/lb for LLDPE (based on CME Globex contracts). Since these price margins do not always exceed the nonethylene cost component of producing PE, the profit margin for converting ethylene into PE appears to be quite low.

Based on these data, we approximated the opportunity cost range for not using ethylene to produce PE as 2−10 cents/lb ethylene, with the specific values of 2, 6, and 10 cents/lb used for the sensitivity study. The sensitivity analysis is done using the same framework as in the previous section, but with the ethylene price fixed at 15 cents/lb and the price of crude oil again fixed at $50/bbl. Results are shown in Figure 12, for the 200 KTA plant capacity (results for 100 KTA are similar and not shown). At the 40% yield to gasoline, the process is adopted only for the 2 cents/lb opportunity cost case and at nonmaterial cost levels below about $195/t gasoline. However, at 60% yield to gasoline, there is adoption even at the 10 cents/lb opportunity cost, with adoption possible over a relatively wide range of nonmaterial cost. From these results, we conclude that even when factoring in the opportunity cost of not producing PE, there is potential for successful adoption

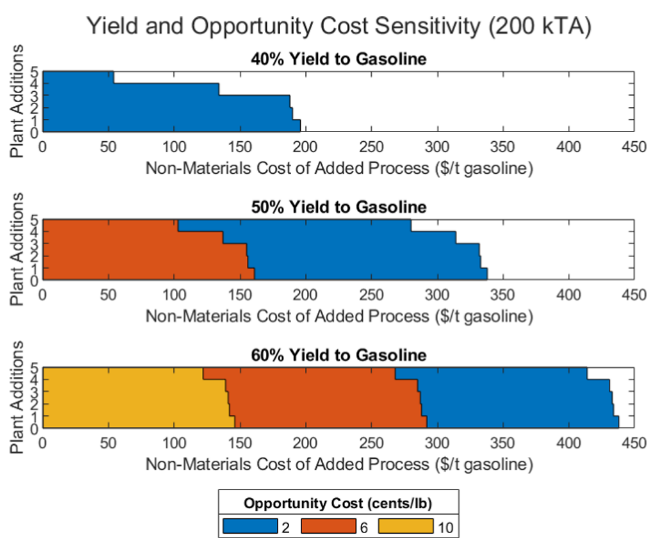

Figure 12. Range of process costs for which the process is viable and the number of plant additions, for different values of opportunity costs and yield to gasoline, for 200 kTA plants.

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of the ethylene to gasoline oligomerization process in a scenario of ethylene overproduction and excess capacity.

5. CONCLUDING REMARKS

In this work, we developed and utilized a new geospatial network model of the U.S. petrochemicals and refining industry, with a focus on the Marcellus Shale region, an area abundant in natural gas liquids (NGLs) and likely future hub for NGL derivatives such as ethylene. The model is a mixed-integer linear program and was used to study the potential for success of new technology for oligomerization of ethylene to gasoline or a gasoline blend stock and to identify the impact this would have on the ethylene supply chain. This was done by applying the model to case studies based on a scenario of ethylene and polyethylene overproduction and excess capacity, a current concern[10] due to the unprecedented growth in ethane cracking capacity. In the case studies, the ethylene oligomerization process was added to the network, and the largest net production cost value at which this technology was adopted into the industry network was determined (maximum adoption cost). These results can be used as benchmarks to assess the oligomerization process under consideration and illustrate a high-level approach for setting cost targets for technology development in the hydrocarbon industry. Furthermore, the optimal locations for the implementation of this technology were identified for each case. Since the model has uncertain parameters, we also employed sensitivity analyses to study the impact of some key parameters, namely, the prices of crude oil and ethylene, the yield to gasoline in the oligomerization process, the oligomerization plant capacity, and the opportunity cost of not producing polyethylene. Overall, this work demonstrates a general geospatial network modeling approach for evaluating new hydrocarbon processing technology and determining its overall impact on the industry.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.1c02300.

Diagram of the workflow used in implementing the model (PDF)

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Notes

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■ NOMENCLATURE

Binary Variable

β_n plant adoption indicator: 1 if plant is chosen, 0 otherwise

Parameters

$a_{C,i}$ number of carbon atoms of product i
$a_{i,j}$ input−output coefficient of material i in technology j
C_n capacity of node $n \in S \cup U \cup Z$
$C_{c,tot}$ total investment capital available
$C_{c,n}$ capital cost of a new plant at node n
$C_{p,n}$ production cost of node n
C_t average cost for truck transportation
D_n production demand for node $n \in K$
$d_{n,m}$ distance between node n and node m
$F^{\circ}_{C_2}$ ethylene molar inlet flow
F_i molar outlet flow of product i
F_{C_2} ethylene molar outlet flow
S_i selectivity to product i

Sets

I all materials
$I_{in,n}$ all input materials i at node n
$I_{out,n}$ all output materials i at node n
J all technologies
K sink nodes
N all network nodes
S supply nodes
U chemical manufacturing unit nodes
Z potential plant nodes

Units

bbl oil barrel = 42 US gallons
KTA thousand metric tons per year
mi mile
MMBTU million BTU
t metric ton

Variables

C_{tot} total annual industry cost
P_n production level of node n

$X_{i,n}$ flow of material i in node n
$Y_{i,n,m}$ magnitude of flow of material i from node n to node m

■ REFERENCES

(1) U.S. Energy Information Administration, U.S. Energy Facts Explained. 2021; https://www.eia.gov/energyexplained/us-energy-facts/imports-and-exports.php, accessed Aug 25, 2021.
(2) Siirola, J. J. The Impact of Shale Gas in the Chemical Industry. *AIChE J.* **2014**, *60*, 810−819.
(3) US Energy Information Administration, Where Our Natural Gas Comes From. 2021; https://www.eia.gov/energyexplained/natural-gas/where-our-natural-gas-comes-from.php, accessed Aug 25, 2021.
(4) U.S. Energy Information Administration, What are natural gas liquids and how are they used? 2012; http://www.eia.gov/todayinenergy/detail.cfm?id=5930, accessed Aug 25, 2021.
(5) Ridha, T.; Li, Y.; Gençer, E.; Siirola, J. J.; Miller, J. T.; Ribeiro, F. H.; Agrawal, R. Valorization of shale gas condensate to liquid hydrocarbons through catalytic dehydrogenation and oligomerization. *Processes* **2018**, *6*, 139.
(6) U.S. Energy Information Administration, Growing U.S. HGL production spurs petrochemical industry investment. 2015; https://www.eia.gov/todayinenergy/detail.php?id=19771, accessed Aug 25, 2021.
(7) Shell Global, Pennsylvania Petrochemicals Complex. 2018; https://www.shell.com/about-us/major-projects/pennsylvania-petrochemicals-complex.html, accessed Aug 25, 2021.
(8) Jordan Blum, DowDuPont opens massive ethylene and plastics plant in Freeport. 2017; https://www.chron.com/business/energy/article/DowDuPont-opens-massive-ethylene-and-plastics-12217420.php, accessed Aug 25, 2021.
(9) Hydrocarbon Processing, Global chemical company starts up ethylene cracker. 2020; https://www.hydrocarbonprocessing.com/news/2020/02/global-chemical-company-starts-up-ethylene-cracker, accessed Aug 25, 2021.
(10) Barrasa, C.; Lewandowski, S.; Cui, T. A door opens: surplus ethylene to gasoline. 2021; https://ihsmarkit.com/research-analysis/a-door-opens-surplus-ethylene-to-gasoline.html, accessed Aug 25, 2021.
(11) Attanatho, L.; Lao-ubol, S.; Suemanotham, A.; Prasongthum, N.; Khowattana, P.; Laosombut, T.; Duangwongsa, N.; Larpkiattaworn, S.; Thanmongkhon, Y. Jet fuel range hydrocarbon synthesis through ethylene oligomerization over platelet Ni-AlSBA-15 catalyst. *SN Appl. Sci.* **2020**, *2*, No. 971.
(12) US Energy Information Administration, How much gasoline does the United States consume? 2021; https://www.eia.gov/tools/faqs/faq.php?id=23&t=10, accessed Aug 25, 2021.
(13) Siluria by Lummus, Ethylene to Liquids. 2020; https://siluria.com/Technology/Ethylene_to_Liquids, accessed Aug 25, 2021.
(14) DeRosa, S. E.; Kimura, Y.; Stadtherr, M. A.; McGaughey, G.; McDonald-Buller, E.; Allen, D. T. Network Modeling of the U.S. Petrochemical Industry under Raw Material and Hurricane Harvey Disruptions. *Ind. Eng. Chem. Res.* **2019**, *58*, 12801−12815.
(15) Stadtherr, M. A.; Rudd, D. F. Systems study of the petrochemical industry. *Chem. Eng. Sci.* **1976**, *31*, 1019−1028.
(16) Stadtherr, M. A.; Rudd, D. F. Resource use by the petrochemical industry. *Chem. Eng. Sci.* **1978**, *33*, 923−933.
(17) Stadtherr, M. A. A systems approach to assessing new petrochemical technology. *Chem. Eng. Sci.* **1978**, *33*, 921−922.
(18) Stadtherr, M. A.; Rudd, D. F. Resource Management in the Petrochemical Industry. *Manage. Sci.* **1978**, *24*, 740−746.
(19) Sophos, A.; Rotstein, E.; Stephanopoulos, G. Multiobjective analysis in modeling the petrochemical industry. *Chem. Eng. Sci.* **1980**, *35*, 2415−2426.
(20) Rudd, D. F.; Fathi-Afshar, S.; Treviño, A. A.; Stadtherr, M. A. *Petrochemical Technology Assessment*; Wiley, 1981; pp 1−157.
(21) Fathi-Afshar, S.; Rudd, D. F. The economic impact of new chemical technology. *Chem. Eng. Sci.* **1981**, *36*, 1421−1425.
(22) Fathi-Afshar, S.; Maisel, D. S.; Rudd, D. F.; Treviño, A. A.; Yuan, W. W. Advances in petrochemical technology assessment. *Chem. Eng. Sci.* **1981**, *36*, 1487−1511.
(23) Fathi-Afshar, S.; Rudd, D. F. Impact of Restrictions on Toxic Substances on The Production of Synthetic Materials. *Polym.-Plast. Technol. Eng.* **1981**, *16*, 99−118.
(24) Fathi-Afshar, S.; Yang, J. C. Designing the optimal structure of the petrochemical industry for minimum cost and least gross toxicity of chemical production. *Chem. Eng. Sci.* **1985**, *40*, 781−797.
(25) Sokić, M.; Zdravković, S.; Trifunović, Z. A multiobjective approach to the structuring of an efficient system for producing petrochemicals from alternative raw materials. *Can. J. Chem. Eng.* **1990**, *68*, 119−126.
(26) Chang, D.; Allen, D. T. Minimizing Chlorine Use: Assessing the Trade-offs Between Cost and Chlorine Reduction in Chemical Manufacturing. *J. Ind. Ecol.* **1997**, *1*, 111−134.
(27) Al-Sharrah, G. K.; Alatiqi, I.; Elkamel, A.; Alper, E. Planning an integrated petrochemical industry with an environmental objective. *Ind. Eng. Chem. Res.* **2001**, *40*, 2103−2111.
(28) DeRosa, S. E.; Allen, D. T. Impact of natural gas and natural gas liquids supplies on the united states chemical manufacturing industry: Production cost effects and identification of bottleneck intermediates. *ACS Sustainable Chem. Eng.* **2015**, *3*, 451−459.
(29) DeRosa, S. E.; Allen, D. T. Impact of New Manufacturing Technologies on the Petrochemical Industry in the United States: A Methane-to-Aromatics Case Study. *Ind. Eng. Chem. Res.* **2016**, *55*, 5366−5372.
(30) DeRosa, S. E. Impact of Natural Gas and Natural Gas Liquids on Chemical Manufacturing in the United States. Ph.D. thesis, The University of Texas at Austin, 2016.
(31) IHS, IHS Process Economics Program Yearbook. 2012; https://ihsmarkit.com/products/chemical-technology-pep-index.html/, accessed Aug 25, 2021.
(32) DeRosa, S. E.; Allen, D. T. Comparison of Attributional and Consequential Life-Cycle Assessments in Chemical Manufacturing. In *Encyclopedia of Sustainable Technologies*; Abraham, M. A., Ed.; Elsevier, 2017; pp 339−347.
(33) Calvo-Serrano, R.; Guillén-Gosálbez, G. Streamlined Life Cycle Assessment under Uncertainty Integrating a Network of the Petrochemical Industry and Optimization Techniques: Ecoinvent vs Mathematical Modeling. *ACS Sustainable Chem. Eng.* **2018**, *6*, 7109−7118.
(34) Leontief, W. W. Input-Output Economics. *Sci. Am.* **1951**, *185*, 15−21.
(35) Mielnik, M.; Ertesva, I. S. Exergy analysis of the Norwegian society. *Energy* **2000**, *25*, 957−973.
(36) Chen, G. Q.; Chen, B. Extended-exergy analysis of the Chinese society. *Energy* **2009**, *34*, 1127−1144.
(37) Horowitz, K. J.; Planting, M. A. Concepts and Methods of the U.S. Input-Output Accounts. 2009; https://apps.bea.gov/papers/pdf/IOmanual_092906.pdf, accessed Aug 25, 2021.
(38) Han, Y.; Liu, S.; Geng, Z.; Gu, H.; Qu, Y. Energy analysis and resources optimization of complex chemical processes: Evidence based on novel DEA cross-model. *Energy* **2021**, *218*, No. 119508.
(39) Wang, Z.; Han, Y.; Li, C.; Geng, Z.; Fan, J. Input-output networks considering graphlet-based analysis for production optimization: Application in ethylene plants. *J. Cleaner Prod.* **2021**, *278*, No. 123955.
(40) Contesse, L.; Ferrer, J. C.; Maturana, S. A mixed-integer programming model for gas purchase and transportation. *Ann. Oper. Res.* **2005**, *139*, 39−63.
(41) Liu, P.; Whitaker, A.; Pistikopoulos, E. N.; Li, Z. A mixed-integer programming approach to strategic planning of chemical centres: A case study in the UK. *Comput. Chem. Eng.* **2011**, *35*, 1359−1373.
(42) Andersen, F.; Iturmendi, F.; Espinosa, S.; Diaz, M. S. Optimal design and planning of biodiesel supply chain with land competition. *Comput. Chem. Eng.* **2012**, *47*, 170−182.

(43) Lara, C. L.; Bernal, D. E.; Li, C.; Grossmann, I. E. Global optimization algorithm for multi-period design and planning of centralized and distributed manufacturing networks. *Comput. Chem. Eng.* **2019**, *127*, 295−310.
(44) Elia, J. A.; Baliban, R. C.; Floudas, C. A. Nationwide, regional, and statewide energy supply chain optimization for natural gas to liquid transportation fuel (GTL) systems. *Ind. Eng. Chem. Res.* **2014**, *53*, 5366−5397.
(45) ICIS, ICIS Supply and Demand Database. 2017; https://www.icis.com/explore/services/analytics/supply-demand-data/icis-supply-and-demand-database/, accessed Aug 25, 2021.
(46) U.S. Bureau of Labor Statistics, CPI Inflation Calculator. 2020; https://www.bls.gov/data/inflation_calculator.htm, accessed 2020-06-16.
(47) Graul, C. leafletR: Interactive Web-Maps Based on the Leaflet JavaScript Library. 2016; http://cran.r-project.org/package/leafletR, R package version 0.4-0, accessed Sep 4, 2021.
(48) OpenStreetMap contributors, Planet dump retrieved from https://planet.osm.org/. 2021; accessed Sep 4, 2021.
(49) Toch, K.; Thybaut, J. W.; Marin, G. B. Ethene oligomerization on Ni-SiO_2-Al_2O_3: Experimental investigation and Single-Event MicroKinetic modeling. *Appl. Catal., A* **2015**, *489*, 292−304.
(50) Toch, K.; Thybaut, J. W.; Arribas, M. A.; Martínez, A.; Marin, G. B. Steering linear 1-alkene, propene or gasoline yields in ethene oligomerization via the interplay between nickel and acid sites. *Chem. Eng. Sci.* **2017**, *173*, 49−59.
(51) Ganesh, H. S.; Dean, D. P.; Vernuccio, S.; Edgar, T. F.; Baldea, M.; Broadbelt, L. J.; Stadtherr, M. A.; Allen, D. T. Product Value Modeling for a Natural Gas Liquid to Liquid Transportation Fuel Process. *Ind. Eng. Chem. Res.* **2020**, *59*, 3109−3119.
(52) US Department of Transportation, Average Freight Revenue. 2019; https://www.bts.gov/content/average-freight-revenue-ton-mile, accessed 2020-02-14.
(53) Magill, J. 2 small-scale gas-to-liquids projects aim for US market. 2018; https://www.spglobal.com/marketintelligence/en/news-insights/trending/WUse9RmGK8u800_su8Lj6A2, accessed Aug 25, 2021.
(54) The General Algebraic Modeling System (GAMS). 2021; https://www.gams.com/, accessed Aug 25, 2021.
(55) Joshi, R.; Saxena, A.; Gounder, R. Mechanistic insights into alkene chain growth reactions catalyzed by nickel active sites on ordered microporous and mesoporous supports. *Catal. Sci. Technol.* **2020**, *10*, 7101−7123.
(56) OPIS Blog by IHS Markit, Ethylene and Propylene Prices in 2020: Two Market Stories. 2020; http://blog.opisnet.com/ethylene-propylene-prices-2020, accessed Aug 25, 2021.
(57) Allen, J. US Plastic Prices Pose Problems. 2015; https://spendmatters.com/2015/05/18/us-plastic-prices-pose-problems/, accessed Aug 25, 2021.