THE FUTURE OF THE CHEMICAL INDUSTRY SHAPED BY GLOBAL CONFLICTS: IMPACT OF MAJOR LNG EXPORTS ON THE U.S. CHEMICAL INDUSTRY

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Abstract

The United States has pledged to help the European Union overcome potential energy shortages, due to loss of Russian oil and gas, by providing additional LNG to European countries. The additional amount exported is planned to be replaced in the U.S. by green energy. However, that process will require time and, therefore, natural gas availability for industrial use in the U.S. may (temporarily) decrease. We present an optimization-based network modeling approach to simulate the U.S. chemical manufacturing and refining industry and to probe the potential impacts of these exports on industry technology choices.

Keywords

Chemical Industry Modeling, LNG, Optimization, Supply Chain

Introduction

Global conflicts can have a significant market impact. Europe has been the epicenter of the latest incarnation of this issue, with the Ukraine conflict leading to sanctions on Russian energy imports and a push for energy independence by the European Union. Replacing the crude oil, natural gas and solid fuel provided by Russia (26.9%, 41.1% and 46.7%, respectively, of total European Union imports in 2019) (Eurostat, 2020) is a strategic process that requires time to complete. The United States has committed to assist this effort by increasing the amount of liquefied natural gas (LNG) that is exported to Germany and other EU countries (Schonhardt, 2022). While LNG export capacity expansion is under way, the current facilities are operating at or near maximum production rates. With natural gas production and LNG liquefaction being potential bottlenecks, the additional 15 billion m^3 (minimum amount) committed by the U.S. (The White House, 2022), for 2022 alone, may be secured by redirecting exports initially meant for other destinations and/or from domestic use (Patel, 2022). Even if natural gas production capacity can be increased to the full extent necessary, it is conceivable that the additional exported amount may reduce the supply of natural gas available to the chemical industry. It is essential to ask “how” and “how much” these strategic commitments will impact the industry, and is precisely these questions that we probe here.

To this end, we employ a network superstructure model (Skouteris et al., 2021), consisting of several hundreds of chemicals and processing technologies, that considers the industry in the entirety of the United States. The model is formulated as an optimization program, seeking to minimize the industry total production cost. First, we establish a base case, using the model to determine the optimal industry configuration based on recent raw material supply and product demand data. Then, we compare the optimal natural gas usage from the base case model to the available natural gas supply for industrial use, with and without the additional LNG exports. Finally, more conservative assumptions on natural gas supplies for industry use are made (i.e., lower availability) and the impact on the industry is discussed.

Chemical Industry Network Modeling

The chemical industry is a complex, interconnected network of material and energy flows that combine in different

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ratios, and collectively are responsible for transforming a relatively small number of feedstock materials into numerous useful chemical and fuel products. There is a wide array of technologies that can be used, depending on feedstock cost and availability, and each technology has different energy usage and costs. Given some overall objective that drives the industry and a specific set of constraints (supply and demand), there exists an optimal industry configuration that represents the ideal set of pathways for the production of the desired products from the available raw materials. This representation of the chemical industry enables the implementation of optimization-based network models, an approach that originated with Stadtherr and Rudd (1976). Network models represent the industry as a directed graph, comprised of nodes corresponding to manufacturing processes and edges that correspond to material and energy flows. Each node represents a processing technology (rather than a specific plant) and is typically characterized by a process stoichiometry and a production cost, while each edge is defined in terms of a material flow rate.

There have been several applications, variations and extensions of this approach over the years, as reviewed by Skouteris et al. (2021) and DeRosa and Allen (2015). Some of the latest examples include assessing the adoption of new technologies into the current industrial network, with a focus on utilizing light alkane resources such as ethane, both regionally (Giannikopoulos et al., 2021) and at a country level (Skouteris et al., 2021). An assessment of the impact on the petrochemicals industry of a significant adoption of green energy and, as a result, a step away from crude oil refining, was also presented (Giannikopoulos et al., 2022). Multi-objective optimization approaches were also developed and used to study the integration of renewable energy sources to chemical manufacturing in an effort to electrify and decarbonize the chemical industry (Giannikopoulos et al., 2022b) and to evaluate the tradeoff between total industry costs and carbon emissions (Giannikopoulos et al., 2022a). Lastly, variable-cost models that account for significant cost changes throughout the network, possibly due to the adoption of new technologies, have also been developed (Skouteris et al., 2021, 2022).

Model Formulation

The current base network model contains 910 processes, 900 materials and 7 utility types (which are used for evaluating process costs). This creates a superstructure of the industry in which all commercially viable manufacturing routes to the desired products are included. Process stoichiometries and costs have been obtained from the IHS 2012 Process Economic Program Yearbook IHS (2012). For the purposes of this study, it is assumed that this information is sufficiently up-to-date. This assumption is based on the fact that major technology changes often take substantial time to develop, and thus this data have likely not changed to a significant extent since 2012. In contrast to smaller industrial networks, the size of the U.S. chemical industry network renders the task of visualizing the graph infeasible.

The model is formulated as an optimization problem whose objective is to minimize the total industry cost, with decision variables being the utilization level X_j of each process technology $j \in J$ in terms of the flow rate of its main product, the exogenous flow rate F_i of material $i \in I$ into the network as a primary feedstock, and the exogenous flow rate Q_i of material $i \in I$ out of the network as a final product, where J is the set of all process nodes and I is the set of all materials. The objective function is the total net industry cost:

$$\min_{X_j, F_i, Q_i} C_{\text{tot}} = \sum_{j \in J} C_j X_j \tag{1}$$

where C_j is the net unit cost of process j (per amount of main product). The net unit processing cost C_j accounts for raw material costs, byproduct credits, and utility costs, and also includes capital investment, expressed as straight-line depreciation over 10-year period, as well as other fixed operating costs (e.g., maintenance, labor, overhead, taxes) based on an average scale plant.

The model also includes material balance and supply and demand constraints. The balance equation for each material i in terms of annual mass flow rates is:

$$F_i + \sum_{j \in J} a_{i,j} X_j - Q_i = 0, \quad \forall i \in I \tag{2}$$

where $a_{i,j}$ is the input-output coefficient for material i in process j (negative if material i is consumed in process j, positive if it is produced; unity if i is the main product of process j). There are also constraints of the amount of materials that enter (supply cannot exceed availability) and exit (production has to exceed demand) the network:

$$0 \leq F_i \leq S_i \tag{3}$$

$$Q_i \geq D_i \geq 0 \tag{4}$$

where S_i is the exogenous supply rate of material i and D_i is the exogenous demand rate of material i.

The linear program (LP) defined by Eqs. (1) – (4) was implemented in the General Algebraic Modeling System (GAMS) (GAMS Development Corporation, 2021) and can be solved by any standard LP solver, such as CPLEX. The solutions are expressed in terms of an industry configuration (i.e., the technologies that are selected for operation) and the magnitudes of the material fluxes between these technology nodes.

Model Application

We apply the model described above to study the potential impact of additional natural gas being exported as LNG from the U.S. to the EU. We consider the following specific questions:

- If the LNG quantities committed for export to the EU were redirected from natural gas supplies usually available to the petrochemicals industry, would this cause any major disruptions in the minimum-cost industry?
- What is the maximum amount of natural gas that could be taken from industry supplies for export as LNG without causing changes in the optimal industry configuration?

- If this maximum amount is exceeded, what are the structural effects on the optimal industry, i.e. what are the industry and technology shifts needed to accommodate the lower natural gas availability?

To address these questions, we formulate and solve three problems:

- Problem A: This problem establishes a base case. The optimization model described above is solved using recent (2019) data for raw material supplies and product demands. There is no reduction of the industry's natural gas supply due to additional LNG exports.

- Problem B: We compare the optimal natural gas usage from the base case model solved in Problem A to the available supply of natural gas for industrial use. The difference in these quantities will establish the maximum amount of natural gas (if unconstrained by LNG liquefaction and export terminal capacity) that could be taken from industry supplies for additional LNG export without inducing changes in the optimal industry configuration. This unconstrained maximum for additional LNG export will be then be compared to the minimum committed case (The White House, 2022) for 2022 of an additional 15 billion m^3 of LNG for the EU, and a maximum constrained case in which all the new LNG terminal capacity projected to come online during 2022 (U.S. Energy Information Administration, 2021b) is used for additional LNG exports.

- Problem C: In this problem, we make more conservative assumptions about the natural gas supplies for industry use. We reduce the supply of natural gas to be less than the natural gas usage in the base case optimal industry of Problem A, thus forcing some adaptation by the industry. We use the model to determine the new optimal industry configuration for different levels of natural gas supply reduction, and see what technological changes occur compared to the base case.

Results from the problems described above are summarized and discussed in the following section.

Discussion

The results from Problems A and B are summarized in Figure 1, which shows LNG export volumes for three different cases. The case labeled "Unconstrained Maximum" corresponds to an excess availability of natural gas in the Problem A base case optimal industry. This represents the amount of LNG that could be produced using this excess natural gas, assuming processing losses of 15% (U.S. Energy Information Administration, 2021a). However, this amount of additional LNG export cannot be actually be realized due to constraints on liquefaction and export terminal capacity. When this capacity constraint is considered the maximum additional LNG export amount for 2022 is 21.7 billion m^3 (bcm), as shown by the "Constrained Maximum" case in Figure 1. The final case shown is the "Committed Minimum" additional LNG to EU export amount of 15 bcm. These comparisons indicate that, at the current additional LNG export levels, there are no disruptions to the minimum-cost petrochemicals industry.

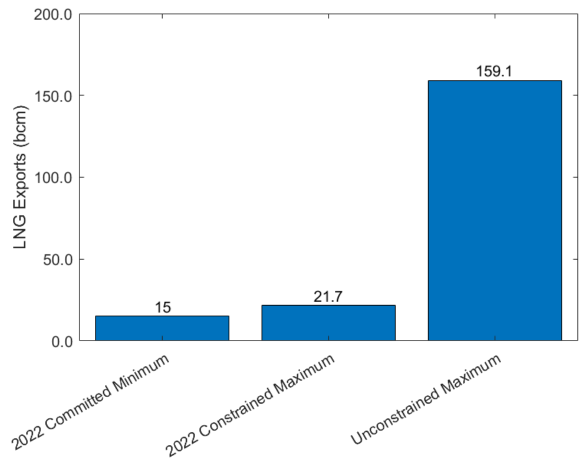

Figure 1: Annual additional LNG exports from U.S. to EU for three cases, in bcm (billions of m^3) (expanded gas basis). See text for discussion.

In Problem C, we have considered the possibility that, as LNG export capacity grows, or if some other pressure arises on natural gas supplies, a situation may arise in which the supply of natural gas to the petrochemicals industry is reduced below its current consumption level in the minimum-cost industry (as determined in Problem A). We considered reductions of 1%, 3% and 5% and determined the structural changes (technology shifts) in the minimum-cost industry needed to accommodate the situation. For the 1% reduction case, the only technology shift that takes place is in the production of ammonia. Part of the ammonia production from methane reforming shifts to a different methane reforming process. The newly adopted process requires smaller amounts of natural gas and comes with a higher production cost, an intuitive result. Similar results are obtained when considering the 3% reduction case, but a greater amount of ammonia production shifts to the more expensive and more methane-efficient process. Reaching the 5% reduction case results in the use of alternative pathways (which are more expensive but use less natural gas) for multiple materials: ammonia, methanol, butadiene, methyl methacrylate, and benzene. A selection of these changes are illustrated in Figure 2. Ammonia production now shifts completely to the UHDE dual pressure process. Methanol also shifts completely from the ICI two-stage reforming process to the methanol on mega scale (reforming) process. Similarly, butadiene completely shifts to a TPC OXO-D process from the catadiene process.

It is important to note that there is uncertainty in several segments of this analysis. Even though some components of processing costs are relatively insensitive to external factors (but are dependent on new technology developments), feedstock prices and supply availability are highly susceptible to supply chain disruptions and, in this case, geopolitical issues. Furthermore, demand (both domestic and international) is generally difficult to predict and can fluctuate. Accounting for such uncertainties, in the context of this and related work, could be addressed using various approaches. For exam-

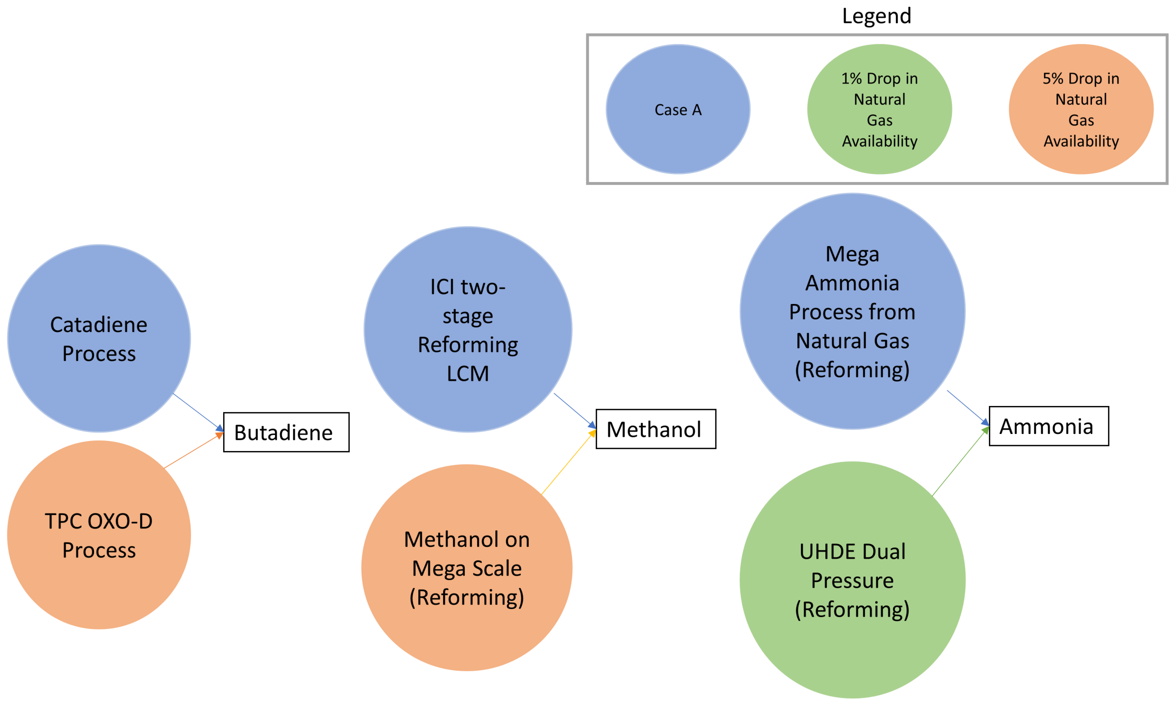

Figure 2: Selected changes in the optimal industry configuration (technology changes) as natural gas supply is reduced below its current consumption level in the minimum-cost industry. Reductions of 1% and 5% shown. A change in a production pathway at 1% drop in availability implies that the same change is present at 5% drop. See text for additional discussion.

ple, optimization under uncertainty (Sahinidis, 2004) and robust optimization (Al-Qahtani et al., 2008) frameworks have been used to describe and quantify uncertainties in this context. Moreover, flexibility metrics and formulations could be used, as seen in various applications in chemical engineering, including supply chain management (Bruns et al., 2020; Swaney and Grossmann, 1985; Di Pretoro et al., 2021; Merschmann and Thonemann, 2011). Such approaches are not used in this current work, but may be implemented in the future.

Conclusions

Through the export of LNG, the United States will play an important role in the efforts of the European Union to become energy independent. This presents significant opportunities for domestic LNG exporters. In this work, we identified the upper limit of additional LNG exports that could be immediately exported without any changes in the structure of the chemical industry, as well as the main technology changes that would be necessary in scenarios with additional LNG exports that go beyond this upper limit and thus reduce natural gas availability to the industry. In future work, we will consider longer-term and more general LNG export commitments, which will require increase of domestic natural gas production with accompanying increases in production of natural gas liquids (NGLs). This latter factor (increasing NGL production) may be an important driver of technological change in the industry.

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References

Al-Qahtani, K., A. Elkamel, and K. Ponnambalam (2008). Robust optimization for petrochemical network design under uncertainty. *Industrial & Engineering Chemistry Research 47*(11), 3912–3919.

Bruns, B., F. Herrmann, M. Polyakova, M. Grünewald, and J. Riese (2020). A systematic approach to define flexibility in chemical engineering. *Journal of Advanced Manufacturing and Processing 2*(4), e10063.

DeRosa, S. E. and D. T. Allen (2015). 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 Chemistry & Engineering 3*(3), 451–459.

Di Pretoro, A., S. Negny, and L. Montastruc (2021). Flexibility analysis in supply chain management: Application to the traveling salesman problem. In M. Türkay and R. Gani (Eds.), *31st European Symposium on Computer Aided Process Engineering*, Volume 50 of *Computer Aided Chemical Engineering*, pp. 1721–1726. Elsevier.

Eurostat (2020). From where do we import energy? https://ec.europa.eu/eurostat/cache/infographs/energy/bloc-2c.html#carouselControls?lang=en. Accessed May 2nd, 2022.

GAMS Development Corporation (2021). The General Algebraic Modeling System (GAMS). https://www.gams.com/. Accessed on 23 July 2021.

Giannikopoulos, I., A. Skouteris, D. T. Allen, M. Baldea, and M. A. Stadtherr (2022a). Multi-objective Optimization of Production Cost and Carbon Loss in the U.S. Petrochemicals Industry. In Y. Yamashita and M. Kano (Eds.), *14th International Symposium on Process Systems Engineering (PSE2021+)*, Volume 49 of *Computer Aided Chemical Engineering*, pp. 547–552. Amsterdam, Netherlands: Elsevier B.V.

Giannikopoulos, I., A. Skouteris, D. T. Allen, M. Baldea, and M. A. Stadtherr (2022b). Network-Based Analysis of Electrified Chemical Processing with Renewable Energy Sources. In L. Montastruc and S. Negny (Eds.), *32nd European Symposium on Computer Aided Process Engineering (ESCAPE32)*, Volume 51 of *Computer Aided Chemical Engineering*, pp. 937–942. Amsterdam, Netherlands: Elsevier B.V.

Giannikopoulos, I., A. Skouteris, T. F. Edgar, M. Baldea, D. T. Allen, and M. A. Stadtherr (2021). Geospatial Network Approach for Assessing Economic Potential of Ethylene-to-Fuel Technology in the Marcellus Shale Region. *Industrial & Engineering Chemistry Research 60*(41), 14801–14814.

Giannikopoulos, I., A. Skouteris, T. F. Edgar, M. Baldea, D. T. Allen, and M. A. Stadtherr (2022). Probing the Impact of an Energy and Transportation Paradigm Shift on the Petrochemicals Industry. *Industrial & Engineering Chemistry Research 61*, 12169–12179.

IHS (2012). IHS Process Economics Program Yearbook. https://ihsmarkit.com/products/chemical-technology-pep-index.html/. Accessed April 5, 2022.

Merschmann, U. and U. W. Thonemann (2011). Supply chain flexibility, uncertainty and firm performance: An empirical analysis of German manufacturing firms. *International Journal of Production Economics 130*(1), 43–53.

Patel, S. (2022). U.S. Agrees to Ramp Up LNG Exports to Europe, Actively Reduce Natural Gas Demand. https://www.powermag.com/u-s-agrees-to-ramp-up-lng-exports-to-europe-actively-reduce-natural-gas-demand. Accessed May 2nd, 2022.

Sahinidis, N. V. (2004). Optimization under uncertainty: state-of-the-art and opportunities. *Computers & Chemical Engineering 28*(6), 971–983.

Schonhardt, S. (2022). The U.S. Will Increase Natural Gas Exports to Europe to Replace Russian Fuel. https://www.scientificamerican.com/article/the-u-s-will-increase-natural-gas-exports-to-europe-to-replace-russian-fuel. Accessed May 2nd, 2022.

Skouteris, A., I. Giannikopoulos, D. T. Allen, M. Baldea, and M. A. Stadtherr (2022). MINLP Framework for Systems Analysis of the Chemical Manufacturing Industry Using Network Models. In L. Montastruc and S. Negny (Eds.), *32nd European Symposium on Computer Aided Process Engineering (ESCAPE32)*, Volume 51 of *Computer Aided Chemical Engineering*, pp. 943–948. Amsterdam, Netherlands: Elsevier B.V.

Skouteris, A., I. Giannikopoulos, T. F. Edgar, M. Baldea, D. T. Allen, and M. A. Stadtherr (2021). Systems Analysis of Natural Gas Liquid Resources for Chemical Manufacturing: Strategic Utilization of Ethane. *Industrial & Engineering Chemistry Research 60*(33), 12377–12389.

Stadtherr, M. A. and D. F. Rudd (1976). Systems study of the petrochemical industry. *Chemical Engineering Science 31*(11), 1019–1028.

Swaney, R. E. and I. E. Grossmann (1985). An index for operational flexibility in chemical process design. part I: Formulation and theory. *AIChE Journal 31*(4), 621–630.

The White House (2022). FACT SHEET: United States and European Commission Announce Task Force to Reduce Europe's Dependence on Russian Fossil Fuels. https://www.whitehouse.gov/briefing-room/statements-releases/2022/03/25/fact-sheet-united-states-and-european-commission-announce-task-force-to-reduce-europes-dependence-on-russian-fossil-fuels. Accessed May 2nd, 2022.

U.S. Energy Information Administration (2021a). Natural gas explained: Liquefied natural gas. https://www.eia.gov/energyexplained/natural-gas/liquefied-natural-gas.php. Accessed April 28, 2022.

U.S. Energy Information Administration (2021b). U.S. liquefied natural gas export capacity will be world's largest by end of 2022. https://www.eia.gov/todayinenergy/detail.php?id=50598. Accessed April 28, 2022.