Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

A Modern Portfolio Theory Approach for Chemical Production with Supply Chain Considerations for Efficient Investment Planning

Mohamad Almoussaoui[a], Dhabia M. Al-Mohannadi[a,b,c]*

[a] Texas A&M University at Qatar, Chemical Engineering Program, Education City, Doha, Qatar
[b] Hamad Bin Khalifa University, College of Science and Engineering, Education City, Doha, Qatar
[c] Texas A&M University, Department of Multidisciplinary Engineering, College Station, Texas, USA
* Corresponding Author: dhabia.al-mohannadi@qatar.tamu.edu.

ABSTRACT

Commodity chemicals and energy supply chains are an essential part of the hydrocarbon industry in several countries. As these supply chains are susceptible to disruptions caused by various risks, the economies of countries that depend on the hydrocarbon sector as a major source of income might be negatively affected. One major risk is the price fluctuations of the resources used in the multiple stages of the supply chains. Investment decisions in this sector aim to secure the investment portfolio's financial returns against the risk of price fluctuations. This work introduces an adaptation of a portfolio optimization technique, the modern portfolio theory (MPT) to the case of commodity chemicals and energy supply chain investments by considering all supply chain stages in formulating the MPT framework. A case study considering four chemical commodities and three potential importing countries is presented with a sensitivity analysis that studies the impact of changing the costs associated with the several stages of the supply chain on the investment portfolio. Results show the importance of integrating both the chemical production and the shipping stages of the supply chain in developing a portfolio optimization framework and its impact on the optimal investment portfolios. The developed model guides investment planners to target the desired financial returns at a minimum risk.

Keywords: Investment Decision, Portfolio Selection, Supply Chain, Modern Portfolio Theory

INTRODUCTION

Since the outbreak of the COVID-19 pandemic, concerns have risen regarding the importance of sustaining energy supply chains to ensure the energy security of importing countries [1] and the financial security of exporting countries [2]. Such supply chains are susceptible to risks such as economic shocks, geopolitical disruptions, pandemics, etc. [3]. The COVID-19 pandemic has caused the highest energy market volatility [4]. It led to a sudden decrease in demand for energy, chronic disruptions to supply chains, and elevated prices after recovery [5]. Similarly, geopolitical acts and threats could drive the risk of a crash in the prices of natural gas and oil [6]. Fluctuations in the prices of the exported commodity chemicals and fuels or the raw materials used in their production can result in increased financial burdens on importing countries or a significant decrease in exporting countries' profits. The hydrocarbon industry contributes significantly to the financial stability of several countries with significant oil and gas reserves. For example, as the hydrocarbon sector has contributed to over 70% of Qatar's government's total revenue and 80% of the country's total exports since 2014 [7], ensuring the security of this sector against the risk of price fluctuations is a priority for the country. The hydrocarbon industry is very capital-intensive, and the budget for some projects is over one billion US dollars [8]. As investments in this sector require large capital, time, and technology investments, selecting investment portfolios is critical [9]. As such, an investment planning methodology is necessary for the hydrocarbon sector in such countries. Optimizing and diversifying the investment portfolio can help decrease the risk of investment return uncertainty resulting from price fluctuations. Diversifying the investment portfolio can ensure the security of the hydrocarbon industry's returns as losses from one investment can be compensated by gains from another and portfolio optimization can help in the investment decision-making process as it aims to maximize a portfolio's expected return while minimizing the uncertainty of the return, the portfolio risk [10]. The Modern Portfolio Theory (MPT) developed by Harry Markowitz is an investment portfolio selection tool that aims to guide an investor in determining the optimal investment portfolio [11]. Markowitz formulated a mean-variance optimization problem that results after its solution in a set of Pareto optimal investment portfolios that maximizes the investment portfolio return for a given level of risk, the efficient frontier. In other words, for a portfolio on the efficient frontier, there is no other portfolio with a higher return for a specified level of risk. The theory has been widely used in several fields as a decision-making tool for investment portfolio selection. The Markowitz framework was adapted to optimize the national grain imports by reducing the cost and risk associated with the imports [12]. Due to the price fluctuations of coal, the theory was used to determine the optimal coal purchasing strategy for Taiwan Power Company [13]. The energy security of energy-importing countries also has been studied extensively using the MPT framework. The impact of the fluctuating prices of oil on China's energy import portfolio was studied [14]. Several research works adapted the MPT framework to problems related to the energy security of the exporter. An MPT framework was developed for investment portfolio diversification of major GCC oil-exporting countries [15]. A similar framework was developed to determine the exporting strategy for a natural gas exporting country [16]. The theory was adopted for selecting investment portfolios for the chemical production industry [17, 18]. The decision-making process of hydrocarbon export investments is based on a complex export system. Investors have several options considering the exported chemical commodities, transportation methods, and partner importers. In other words, the problem is of a supply chain scope. The previous adaptations of MPT to the chemical exports problem had several drawbacks: either the development of the framework did not consider a supply chain perspective ignoring the importance of selecting not only the exported commodities but also the partner importers or did not consider the foundations of chemical production and transportation processes This is reflected by disregarding the price fluctuations of all raw materials and utilities used in the export system and considering the price uncertainty of the traded commodities only. A visual representation of the hydrocarbon export problem and the associated price fluctuations is shown in Figure 1. For an exporting country, considering both the production and transportation stages affects the efficient frontier, the set of optimal investment portfolios. To counter the risk of price fluctuations associated with the hydrocarbon exports investments problem, this work develops an MPT framework by considering a supply chain perspective and the foundations of chemical production and transportation as a tool to aid investors in the investment decision-making process. Two efficient frontiers are obtained after solving the Markowitz optimization problem, the first by considering the production stage of the supply chain only and the second by considering both the production and transportation stages.

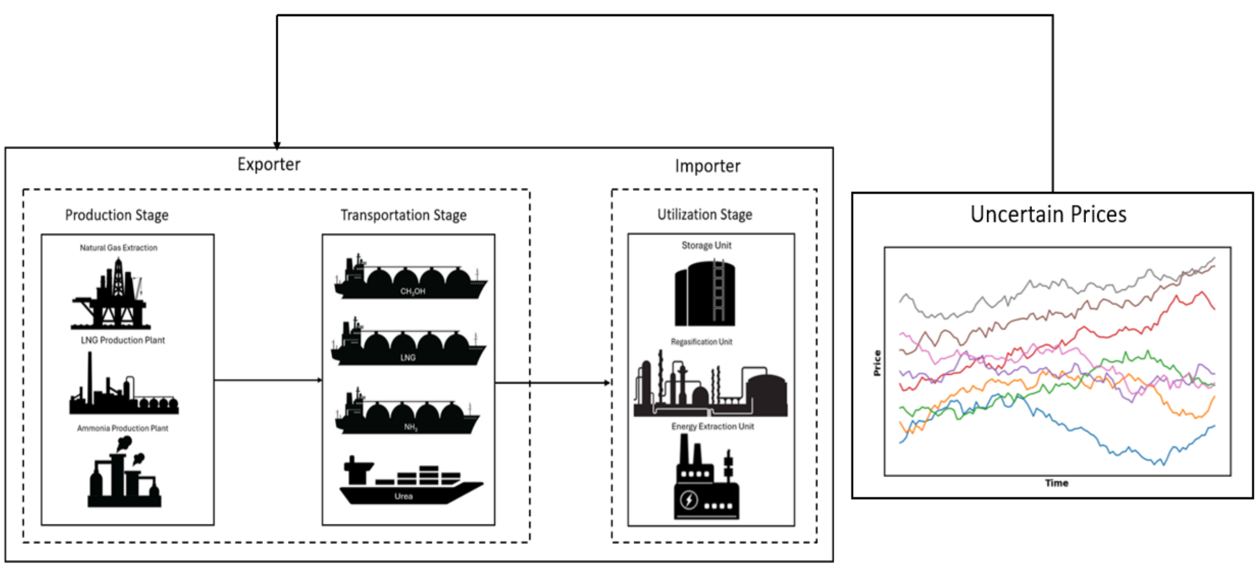

Figure 1: The price uncertainty associated with a hydrocarbon export system.

APPROACH AND PROBLEM STATEMENT

The work aims to develop an MPT framework for energy and commodity chemicals supply chain investments, to determine the investment portfolios with the maximum financial returns at a given level of risk.

Given is a set of commodity chemicals $C = \{c_1, c_2, ..., c_n\}$, $n \in \mathbb{N}$ each produced by a respective production plant from the set $P = \{p_1, p_2, ..., p_n\}$, $n \in \mathbb{N}$. Let $I = \{I_{i,1}, I_{i,2}, ..., I_{i,k_i}\}$, $k_i \in \mathbb{N}$, be the set of potential importing countries of the commodity chemical c_i where k_i is the total number of potential importing countries of c_i. $I_{i,j}$ is the j-th importing country of the chemical c_i where $j = 1, 2, ..., k_i$. A supply chain is defined as a combination of a commodity and an importing country. It is represented as $S_{ij} = \{(c_i, I_{i,j})\}$ where i is the index referring to the traded commodity and j is the index referring to the importer of the commodity. The weight of the capital invested in the supply chain asset $S_{i,j}$ is $w_{i,j} \in [0,1]$. The resulting supply chains represent the potential investment assets constituting an investment portfolio. The historical price data for the production plants' inputs and outputs are required. The plant inputs are the raw materials and energy requirements needed to produce the commodity chemical c_i, and the latter is the plant output. Further information on the plants' capital, fixed, and variable operating costs is required. Such data ensures the ability to determine the efficient frontier for a chemical production investment problem. Additionally, a transportation mode to export the commodity c_i to the importing country I_i is defined. Information on the distance between the exporter and the importer, the transporting ship type, its speed, capital cost, the bunker fuel, its consumption rate, and cost is required. This information is needed to account for the transportation stage of the supply chain. The total amount of capital to be invested in the supply chain portfolio is given. To be calculated is the return on each supply chain investment over a given period. The variance of the return due to fluctuation of the prices of the supply chain inputs and outputs is calculated over a given period. The standard deviation represents the risk of investing in the asset.

The optimization problem is once formulated considering the production stage of the supply chain only and then by additionally accounting for the transportation stage. Evaluating the optimization problem results in determining the efficient frontier that shows the constituting supply chain investments of an optimal portfolio, their respective return and risk, and the weight of capital allocated for each supply chain investment. The weight reflects the capacity of each production plant p_i and the amount of the commodity c_i that should be exported to the importer I_i, using the specified transportation method. The efficient frontier is generated for both cases. The difference between the two obtained efficient frontiers emphasizes the importance of using a supply chain perspective to address the hydrocarbon exports investment selection problem.

A sensitivity analysis is conducted by varying the cost of producing or transporting a commodity, c_i, to study the impact of such changes on the efficient frontier's constituting portfolios. The sensitivity analysis can reflect the effect of using new technologies in producing and transporting chemical commodities on the optimal investment portfolios.

METHODOLOGY

The starting point for formulating the model is the general MPT concepts and equations [19]. Adapting the MPT framework to the commodity chemicals supply chain problem requires calculating each investment portfolio's return and risk. This requires calculating the return on each supply chain investment, $ROI_{supply\ chain,\ year}$, by considering the yearly profit of the supply chain, $Profit_{supply\ chain,\ year}$, and the total capital cost of the supply chain investment, $Capital\ Cost_{supply\ chain,\ year}$, which are variable over time due to fluctuations in prices as shown in Equation 1:

$$ROI_{supply\ chain,year} = \frac{Profit_{supply\ chain,year}}{Capital\ Cost_{supply\ chain,year}}\ \forall\ supply\ chain \tag{1}$$

The profit of the supply chain is the supply chain revenue from the sales of the chemical commodity, $Revenue_{supply\ chain}$, after deducting the fixed and variable operating costs and the cost of depreciation designated as $Fixed\ OPEX_{supply\ chain}$, $Variable\ OPEX_{supply\ chain}$, and $Depreciation_{supply\ chain}$, respectively, as shown in Equation 2:

$$Profit_{supply\ chain} = Revenue_{supply\ chain} - Fixed\ OPEX_{supply\ chain} - Variable\ OPEX_{supply\ chain} - Depreciation_{supply\ chain}\ \forall\ supply\ chain \tag{2}$$

However, since it is assumed that the exporter is responsible for the production and shipping stages of the supply chain, both stages contribute to cost calculation as shown in Equation 3, Equation 4, and Equation 5:

$$Fixed\ OPEX_{supply\ chain} = Fixed\ OPEX_{supply\ chain}{}^{Production} + Fixed\ OPEX_{supply\ chain}{}^{Shipping}\ \forall\ supply\ chain \tag{3}$$

Where $Fixed\ OPEX_{supply\ chain}{}^{Production}$ and $Fixed\ OPEX_{supply\ chain}{}^{Shipping}$ designate the fixed operating costs of the production plant and transporting ship, respectively, accounting for labor and maintenance costs. In Equation 4, $Variable\ OPEX_{supply\ chain}{}^{Production}$ and $Variable\ OPEX_{supply\ chain}{}^{Shipping}$ designate the variable operating costs of the production plant and transporting ship, respectively. These include the variable costs of raw materials and utilities required for the processing plants and the cost of shipping fuel.

$$Variable\ OPEX_{supply\ chain} = Variable\ OPEX_{supply\ chain}{}^{Production} + Variable\ OPEX_{supply\ chain}{}^{Shipping}\ \forall\ supply\ chain \quad (4)$$

In Equation 5, $Depreciation_{supply\ chain}{}^{Production}$ and $Depreciation_{supply\ chain}{}^{Shipping}$ designate the costs resulting from the depreciation of the production plant and transporting ship, respectively.

$$Depreciation_{supply\ chain} = Depreciation_{supply\ chain}{}^{Production} + Depreciation_{supply\ chain}{}^{Shipping}\ \forall\ supply\ chain \quad (5)$$

Similarly, the capital cost of a supply chain is the sum of the capital cost of the production plant, $Capital\ Cost_{supply\ chain}{}^{Production}$, and that of the transporting ship, $Capital\ Cost_{supply\ chain}{}^{Shipping}$, as shown in Equation 6:

$$Capital\ Cost_{supply\ chain} = Capital\ Cost_{supply\ chain}{}^{Production} + Capital\ Cost_{supply\ chain}{}^{Shipping}\ \forall\ supply\ chain \quad (6)$$

The weight of the investment capital allocated to each supply chain investment is denoted as $w_{supply\ chain}$. The return of a portfolio, Portfolio Return, is defined as a weighted average of the average return of a supply chain investment over the years, $\overline{ROI_{supply\ chain}}$:

$$Portfolio\ Return = \sum_{supply\ chain} w_{supply\ chain} \times \overline{ROI_{supply\ chain}} \quad (7)$$

The variance of a portfolio is determined as follows:

$$Portfolio\ Variance = \sum_{supply\ chain} w_{supply\ chain} \times Variance\ ROI_{supply\ chain} + 2\sum_{supply\ chain} \frac{\rho_{ROI_{supply\ chain}, ROI_{supply\ chain+1}}}{SD_{supply\ chain} SD_{suply\ chain+1}} \quad (8)$$

Where $\rho_{ROI_{supply\ chain}, ROI_{supply\ chain+1}}$ is the correlation coefficient between the returns of two supply chain investments and $SD_{supply\ chain}$ is the standard deviation of the investment return. The risk of a portfolio, Portfolio Risk, is defined as the standard deviation of the portfolio's variance:

$$Portfolio\ Risk = \sqrt{Portfolio\ Variance} \quad (9)$$

After developing an MPT framework for the commodity chemicals and energy supply chain problem, the multi-objective optimization problem is presented as follows:

$$\begin{aligned} &Maximize\ Portfolio\ Return \\ &Minimize\ Portfolio\ Risk \\ &Subject\ to\ \textstyle\sum_{supply\ chain} w_{supply\ chain} = 1 \end{aligned} \quad (10)$$

The problem evaluation results in determining the efficient frontier, a set of Pareto optimal investment portfolios.

As a plant can produce a commodity exported to multiple countries and a ship can transport the commodity to several destinations, an investor should aim for the least number of processing plants and transporting ships required which is considered in the developed model. Moreover, as the supply chains are defined specifically with a single importing country, the capital cost associated with the production and transportation stages of the supply chain is calculated based on the demand share of the importing country.

CASE STUDY

A case study is designed to test the developed methodology. The four commodities considered in the case study are methanol, ammonia, urea, and LNG, all of which can be produced from natural gas. It is assumed that the exporter is a country in the Middle East with abundant natural gas reserves and the considered importers are India, China, and Singapore. Chemical commodities are to be transported to destinations using ships. The case study considers 12 possible supply chain investments, which is the maximum number of possible combinations of commodities and importing countries. These supply chains are: (Methanol, India), (Methanol, China), (Methanol, Singapore), (Ammonia, India), (Ammonia, China), (Ammonia, Singapore), (Urea, India), (Urea, China), (Urea, Singapore), (LNG, India), (LNG, China), and (LNG, Singapore). The work will be based on the period between 2018 and 2023. The import demand of the countries for these chemical commodities from the exporter is obtained from the World Integrated Trade Solution database of the World Bank [20]. The historical prices of raw materials, utilities, and exported commodities obtained from the Intratec database were used in this case study [21]. After calculating the return on each supply chain investment and its associated risk, the multi-objective optimization problem presented by Equation 10 is solved twice to determine the efficient frontier: first by considering only the costs of the production stage of the supply chain and then by considering the costs associated with both the production and shipping stages. Hence, two efficient frontier curves are determined. Python's Gurobi solver was used to evaluate the optimization problem using the epsilon constraint method [22].

While Figure 2 shows the efficient frontier determined only when considering the production stage of the supply chain, Figure 3 shows the efficient frontier determined when considering both the production and transportation stages. The constituting investment portfolios of the efficient frontier curves of Figure 2 and Figure 3 are shown in Table 1 and Table 2 respectively.

As shown, developing an MPT framework based on all supply chain stages increased the number of optimal portfolios from five to seven, decreased the maximum possible return due to accounting for transportation costs, and decreased the portfolio risk range due to the increased diversification of the investment portfolios. The constituting supply chains of the optimal portfolios differ between the two efficient frontier curves obtained due to the effect of transportation costs in altering the attractiveness of the supply chain investments. The number of optimal assets in the optimal portfolios of the efficient frontier developed based on the production stage only ranged between one and three. However, introducing a supply chain perspective while developing the MPT framework increased this number where it ranged between one and nine. As such, a supply chain perspective offers a larger number of optimal investment export portfolio options. The portfolio with the highest return in both cases is a one-asset portfolio. It is the supply chain exporting methanol to Singapore which is the asset with the highest return on investment.

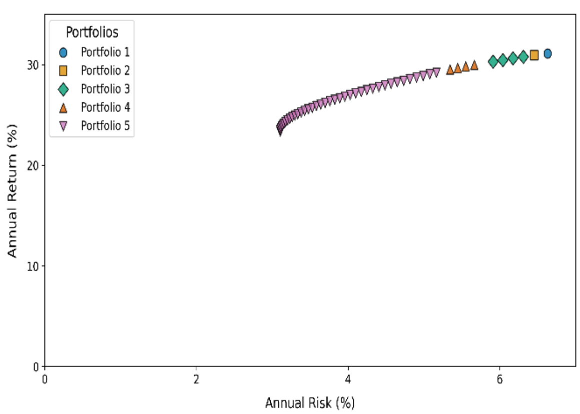

Figure 2: Commodity chemicals and energy production processes efficient frontier.

Table 1: The constituting investments of the commodity chemicals and energy production processes efficient frontier

Portfolio	Constituents
Portfolio 1	(Methanol, Singapore)
Portfolio 2	(Methanol, China), (Methanol, Singapore)
Portfolio 3	(Methanol, China), (Methanol, Singapore), (LNG, China)
Portfolio 4	(Methanol, Singapore), (LNG, China)
Portfolio 5	(Methanol, Singapore), (Urea, China), (LNG, China)

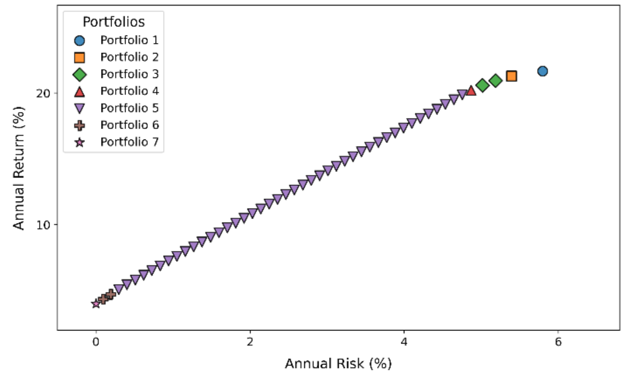

Figure 3: Commodity chemical and energy supply chains efficient frontier.

Table 2: The constituting investments of the commodity chemicals and energy supply chains efficient frontier.

Portfolio	Constituents
Portfolio 1	(Methanol, Singapore)
Portfolio 2	(Methanol, India), (Methanol, Singapore)
Portfolio 3	(Methanol, India), (Methanol, China), (Methanol, Singapore), (Ammonia, India)
Portfolio 4	(Methanol, China), (Methanol, Singapore), (Ammonia, India)
Portfolio 5	(Methanol, China), (Methanol, Singapore), (Ammonia, India), (Urea, India), (Urea, China)
Portfolio 6	(Methanol, China), (Methanol, Singapore), (Ammonia, India), (Urea, India), (Urea, China), (Urea, Singapore)
Portfolio 7	(Methanol, India), (Methanol, China), (Methanol, Singapore), (Urea, India), (Urea, China), (Urea, Singapore), (LNG, India), (LNG, China), (LNG, Singapore)

While LNG production was a constituent of three out of five optimal portfolios in the chemical production efficient frontier, it is only a constituent of one portfolio in the supply chain perspective efficient frontier, the portfolio with the lowest risk. This is a result of the high transportation costs associated with LNG shipping. Methanol was present in all optimal portfolios of the two efficient frontier curves as investments in methanol exports are of the highest return. The production of ammonia is not considered an attractive investment based on the production stage efficient frontier. Similarly, urea is only present in Portfolio 5 of the production stage efficient frontier due to the lower return of this commodity compared to methanol and LNG. For the supply chain perspective efficient frontier, the first two portfolios with the highest returns include only methanol supply chains. The export of ammonia and urea becomes attractive for portfolios of lower risk and return. The general trend in both cases is that decreasing the risk requires increasing the number of portfolio constituents which reflects the ability of portfolio diversification to decrease the return uncertainty, the investment portfolio risk.

The sensitivity analysis considers four alterations of the base case: twice by decreasing the production capital costs of the considered commodities, and twice by decreasing the shipping capital costs. The analysis shows that reducing all commodities' production or transportation costs increases the number of optimal supply chain portfolios as shown in Table 3. As such, using technologies with lower costs will increase the number of options an investor can consider. The constituting optimal supply chains of the five cases considered in the sensitivity analysis were different. While in the base case supplying LNG to India was an optimal investment in one portfolio only, reducing the transportation cost by 20% made this investment present in five optimal portfolios increasing its attractiveness.

Table 3: The impact of the changes in the cost on the number of optimal supply chain investment portfolios

Case	Number of Optimal Portfolios of the Efficient Frontier
Base case	7
20% decrease in production costs	11
80% decrease in production costs	12
20% decrease in transportation costs	11
80% decrease in transportation costs	11

CONCLUSION

In response to the risk of price fluctuations affecting the financial security of hydrocarbon commodities exporters, a framework of MPT, an investment portfolio selection tool, has been developed for the energy and commodity chemicals supply chain problem. The developed model can determine the optimal investment options in terms of the traded commodities, capacities of production plants, partner importers, and the supply volume to each country. As the previous adaptation of MPT to the hydrocarbon exports field did not consider either a supply chain perspective or was not developed based on chemical production and transportation foundations, this work shows the impact of using a supply chain perspective in developing an MPT framework on the portfolio selection process. The developed MPT framework was applied to a case study by considering four commodities with their respective transportation modes and three potential importing countries. The results suggest that the developed framework can provide additional insight into what previous work has shown and act as a decision-making tool to aid investors in the commodity chemicals and energy export sector.

ACKNOWLEDGEMENTS

The authors have no acknowledgments to disclose.

REFERENCES

1. Liu, S.Q., Huang, X., Li, X., Masoud, M., Chung, S., Yin, Y. How is China's energy security affected by exogenous shocks? Evidence of China-US trade dispute and COVID-19 pandemic. *Discov Energy* 1 (2021). https://doi.org/10.1007/s43937-021-00002-6
2. Szczygielski, J. J., Brzeszczyński, J., Charteris, A., Bwanya, P. R. The COVID-19 storm and the energy sector: The impact and role of uncertainty. *Energy Econ.* 109 (2022). https://doi.org/10.1016/j.eneco.2021.105258
3. Energy Technology Perspectives 2023. International Energy Agency (2023).
4. Shaikh, I. Impact of COVID-19 pandemic on the energy markets. *Econ Change Restruct* 55: 433–484 (2021). https://doi.org/10.1007/s10644-021-09320-0
5. Energy Technology Perspectives 2024. International Energy Agency (2024).
6. Apergis, N., Fahmy, H. Geopolitical risk and energy price crash risk. *Energy Econ.* 140 (2024). https://doi.org/10.1016/j.eneco.2024.107975
7. International Trade Administration https://www.trade.gov/country-commercial-guides/qatar-market-challenges.
8. Bret-Rouzaut, N. Economics of Oil and Gas Production. In The Palgrave Handbook of International Energy Economics. Palgrave Macmillan Cham, (2022).
9. Lin, Z., Ji, J. The portfolio selection model of oil/gas projects based on real option theory. *ICCS* (2007). https://doi.org/10.1007/978-3-540-72588-6_151
10. Markowitz, H. M. Portfolio Selection: Efficient Diversification of Investments. Yale University Press (1971).
11. Markowitz, H. PORTFOLIO SELECTION*. *J. Finance* 7: 77-91 (1952). https://doi.org/10.1111/j.1540-6261.1952.tb01525.x
12. Karakoc, D.B., Konar, M. Optimization of national grain imports to balance risk and return: a portfolio theory approach. *Environ. Res.: Food Syst.* 1

(2024). https://doi.org/10.1088/2976-601X/ad22d1
13. Huang, Y.-H., Wu, J.-H. A portfolio theory based optimization model for steam coal purchasing strategy: A case study of Taiwan Power Company. *J. Purch. Supply Manag.* 22: 131-140 (2016). https://doi.org/10.1016/j.pursup.2016.03.001
14. Wu, G., Liu, L.-C., Wei., Y.-M. Comparison of China's oil import risk: Results based on portfolio theory and a diversification index approach. *Energy Policy* 37:3557 - 3565 (2009). https://doi.org/10.1016/j.enpol.2009.04.031
15. Bollino, C. A., Galkin, P. Energy security and portfolio diversification: conventional and novel perspectives. *Energies* (2021). https://doi.org/10.3390/en14144257
16. Nowrouzi, A., Panahi, M., Ghaffarzadeh, H., Ataei., A. Optimizing Iran's natural gas export portfolio by presenting a conceptual framework for non-systematic risk based on portfolio theory. *Energy Strat. Rev.* 26 (2019). https://doi.org/10.1016/j.esr.2019.100403
17. Shehab, S., Al-Mohannadi, D.M., Linke, P. Chemical production process portfolio optimization. *Chem. Eng. Res. Des.* 167: 207-217 (2021). https://doi.org/10.1016/j.cherd.2021.01.013
18. Shehab, S., Linke, P., Al-Mohannadi, D.M. Chemical production process portfolio optimization considering resource integration. *Chem. Eng. Res. Des.* 179: 285-297 (2022). https://doi.org/10.1016/j.cherd.2022.01.022
19. J. C. Francis and D. Kim, Assessing Risk. In: Modern Portfolio Theory: Foundations, Analysis, and New Developments. John Wiley & Sons, Incorporated (2013)
20. World Integrated Trade Solution. https://wits.worldbank.org/.
21. Intratec. https://www.intratec.us/.
22. Gurobi Optimization. https://www.gurobi.com/