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Data-Driven Decision-Making for Flexible Natural Gas Allocation Under Uncertainties: An Agent-Based Modelling Approach

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ABSTRACT

Despite the anticipated growth in the global demand for energy commodities, the frequently changing market dynamics imposed by environmental regulations and political sanctions create end-user demand uncertainties. This imposes the need for prompt quantitative decision-making approaches to understand how various market structures affect the planning of current natural gas projects. Agent-based modelling (ABM) emerges as a powerful approach to facilitate expedited and well-informed decisions amidst limited timeframes. This study deploys agent-based modelling to investigate natural gas allocation across various utilisation routes under diverse economic and environmental scenarios. Results from four main cases and two sub-scenarios imply that the allocation strategy is driven by utilisation routes considered in each case, followed by the allocation target (i.e., economic or environmental) and the operational bounds. The results reveal that cases prioritising natural gas monetisation for export outperform those meeting power requirements in average annual profitability. In case 4, considering a full network with power, the average annual profitability in the economic scenario reduces by approximately 47% compared to case 3, representing the optimal network configuration with $5.22 billion in average annual profitability. However, the economic scenario of case 3 demonstrates the second-highest rate of emissions (0.66 CO_2-eq t/y), following the hydrogen-rich process routes in case 2. Overall, this study presents an innovative data-driven framework for enhancing strategic resource allocation in dynamic business environments. By integrating empirical evidence and technical data with an advanced technical tool (i.e., ABM), the framework provides decision-makers and policymakers with valuable insights for managing uncertainties and shifts in market structures, particularly in existing natural gas projects.

1. Introduction

Supported by the population and economic growth, the global demand for energy commodities is anticipated to grow rapidly [1]. While the increased demand for energy commodities draws greater prosperity to exporting nations, changing market policies generates new challenges. From a supplier perspective, the shifts in the energy markets in the short period between 2020 and 2023 were demonstrated by a transition from challenges in securing markets to challenges in meeting the demand of different segmented markets [2]. For example, the state of Qatar, a major LNG supplier, was motivated to seize mid-term demand opportunities in Europe by the acquisition of LNG regasification terminals in the continent to increase its market share. Yet, with increased uncertainties in the final markets, suppliers must efficiently decide on optimal natural gas monetisation routes and production capacities. One of the fundamental strategies to minimise risks has been production portfolio diversification, wherein several chemical and physical natural gas monetisation options have been deployed in countries with rich natural gas reserves for export purposes since the last century. Monetisation options, such as liquified natural gas, gas-to-liquids, compressed natural gas, and gas-to-chemicals, including methanol and ammonia, have dominated natural gas portfolios.

Each exporting country has a distinct natural gas supply chain shaped by the nature of its gas reservoirs and the market it serves [3]. Consequently, as the complexity of end markets increases, exporting nations must optimise the efficiency of their existing natural gas supply chains. While robust operations have been significant in tackling internal uncertainties impacting natural gas projects, flexible operations have grown as an area of interest in the last few years. Emerging for the “real-options” theory in finance, a flexible system allows the decision-maker to adjust the production capacity depending on the consumer behaviour in the final markets. At increased demand or prices, a

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producer has the option, but not the obligation, to increase the production capacity and capture market opportunities, while the producer also has the right to reduce the production capacity at lower market conditions. Flexibility in operations is associated with technical limitations and constraints, including operational limits, resource availability, and added costs. Hence, understanding the technical capabilities of existing systems in switching production capacities is essential in the early design stages for optimal decision-making. Once the technical limitations are determined, quantitative decision-making tools are used to evaluate the impact of varied forecasted demand and prices on the production levels of different natural gas-based commodities.

Agent-based modelling (ABM) has been identified as a powerful quantitative tool for decision-making in the energy industry. In the context of complex multi-energy systems, the tool has been used for production–distribution planning [4,5], stakeholder engagement [6], and policy-making [6], stimulating interactions of diverse actors like producers, consumers, and regulators. Unlike traditional models, ABM captures emergent behaviours and non-linear dynamics, making it ideal for analysing complex systems. It allows for scenario analysis and policy evaluation by incorporating real-world decision-making rules, aiding in understanding market fluctuations, technology adoption, and regulatory impacts. This makes ABM crucial for optimising energy systems and supporting the transition to sustainable energy, as demonstrated in recent resource network allocation studies for production portfolio optimisation [5,7,8]. The work presented herein discusses the utilisation of ABM as a decision-making tool for optimising natural gas to different downstream processes in Qatar as a response to demand fluctuations in global markets. Considering operational flexibility, the quantitative tool utilises techno-economic and environmental data as inputs to decide on the most economic or environmentally-friendly annual allocation strategy based on market performance.

1.1. Literature review

Qualitative and quantitative decision-making tools have acquired a significant interest in the literature and industry to ensure efficient decision-making based on social, economic, environmental and technical criteria [9–12]. Energy-based studies reported tools for decision-making at different strategic, tactical, and operational levels and ranged from individual to international domains depending on the problem. Consequently, approaches such as multi-decision-criteria decision-making (MCDM), game theory, SWOT analysis, financial analysis, break-even analysis, decision trees, and operations research have been implemented for informed decision-making based on the problem's context [10,13]. Among these, MCDM tools have been particularly prominent in energy planning and assessment. Nasrollahi et al. [14] developed a framework using a multi-criteria decision-making approach comprising 20 options and 52 criteria for selecting wave energy technologies for electricity generation as alternatives to green technologies. The developed framework was utilised for a case study in the Caspian Sea, Iran, to select the optimal option using the outranking model, PROMETHEE, developed by Brans et al. [15] for ranking the alternatives. While other techniques have been observed in the literature, including value measurement methods and goal or reference level models, the PROMETHEE technique has been the most common approach in energy management problems due to its ability to handle both qualitative and quantitative criteria [16–18]. Additionally, MCDM tools have been applied in regional energy systems planning, such as in the UK [19], Ghana [20], Pakistan [21], Algeria [22], and Turkey [23].

Furthermore, MCDMs have been integrated with other tools to overcome limitations. For example, given the literature suggestions of the SWOT analysis weakness in identifying and evaluating factors, Almutairi et al. [13] investigated optimal renewable energy growth strategies in Iran using a combination of three approaches: SWOT analysis, hybrid MCDM method, and game theory. The approach was reported to be novel in considering grey numbers and the SWARA and ARAS methods to eliminate uncertainty in evaluating SWOT analysis factors. Additionally, game theory was used to overcome the weakness of SWOT analysis and MCDM methods in assessing the dependence between strategic factors. Overall, the literature search mainly suggested that MCDM tools have been primarily used to evaluate and assess deployment and implementation alternatives. Sahoo and Goswami [24] concluded that MCDM tools are inadequate for decision-making under uncertainty and demonstrate complexity in stakeholder involvement in the decision-making process. This, in turn, highlighted the need for user-friendly interfaces in industrial applications.

While MCDM tools qualitatively address technical aspects, limited studies focused on techno-economic frameworks for managing existing infrastructure based on market requirements. This gap highlights the need for dynamic models, particularly in planning under uncertainty, where proactive decisions can respond to changes in input parameters. Simulation-based approaches, including mathematical optimisation and agent-based modelling, have proven effective in managing and retrofitting existing projects. To address environmental pollution and stakeholders' conflicts in integrated energy systems, Wang et al. [25] proposed a collaborative optimisation approach for optimal management. Following a three-step framework, the authors introduced a novel multistakeholder low-carbon transaction mechanism, a reward-punishment carbon trading mechanism, and an integrated demand response strategy. Mathematical models for stakeholders were solved with a two-stage optimisation algorithm, demonstrating that the proposed strategy optimally schedules the integrated energy system in a carbon-constrained environment, benefiting all stakeholders economically and environmentally.

At a regional level, Mostatazadeh et al. [26] proposed a multi-objective mathematical model for optimising the energy retrofit of a residential building in Iran, accounting for various future climate and energy price scenarios. Horasan et al. [27] employed a multi-objective model to evaluate renewable energy options for electricity generation in Turkey using a multi-objective mathematical model. The authors assessed solar, wind, geothermal, biomass, and hydroelectric resources across 21 distribution zones to balance social, economic, and environmental objectives. Using a two-phase fuzzy goal programming approach, the model sought to minimise environmental impact and total cost while maximising technical performance and job creation. Multi-objective models have also been applied to energy portfolio planning for better decision-making and policy formulation [28–31]. A recent study by Selçuklu et al. [32] addressed long-term electricity generation planning in Turkey under uncertainty using a multi-objective genetic algorithm and Pareto Uncertainty Index. Overall, mathematical programming-based tools have been effective in optimising energy systems under demand uncertainties. However, they involve lengthy modelling and implementation times, lack flexibility, and may require specialised algorithms for certain scenarios. Therefore, Agent-Based Modeling (ABM) has emerged as a valuable tool for managing existing energy systems under various scenarios, offering both effectiveness and faster implementation.

Originating in the 1970's to study social segregation and cooperation in the social sciences, ABM later emerged in ecology as "individual-based modelling" to simulate ecological population processes involving decisions like movement, feeding, and social interactions [33–36]. However, the underlying principles of the decision-making process in ecology were associated with challenges in integration in the classical models. Previous individual-focused models with simple decision rules yielded valuable insights but have not captured real decision-making complexities. The resultant actions did not represent the actual approaches to making real-life decisions. This is due to the fact that environmental factors, internal states, imperfect knowledge, and social aspects influence decisions. Following this tradition, ABM acquired significant attention in energy, healthcare, and technology due to the tool's capability to provide a solution and allow for a detailed depiction of decision processes by evaluating the impact of the action taken in minute detail [37]. Contemporary ABMs can replicate thousands of individuals in realistic settings, featuring complex internal physiology and perception. Moreover, they allow individuals to process perceptions and make decisions based on internal states, using decision-making methods that range from simple logical rules to advanced neural networks and genetic algorithms. In the literature, several review studies discussed ABM as a decision-making approach in various domains [37–39].

With increased complexities in the energy market dynamics in the last two decades, ABM emerged as a powerful and flexible tool for investigating the interactions between energy producers, retailers, consumers, and regulators. ABM applications in the energy domain included optimal investment, scheduling, production, and distribution decisions at strategic, tactical, and operational planning horizons. In energy retail markets and portfolio management, ABM enables the simulation of different retailer strategies, pricing mechanisms, and market dynamics, allowing decision-makers to assess competition impacts. For example, in retail electricity markets, retailers sign bilateral contracts with end-users to hedge against price volatility, often involving high premiums to mitigate high market risks. A study by Algarvio & Lopes [40] utilised the agent-based simulation tool, Multi-Agent Trading Electricity Markets (MATREM), to optimise retailers' portfolios by implementing 6 retailer agents with individual risk preferences and 312 end-consumers in the Iberian market (i.e. Portugal and Spain).

In industrial enterprises, Budinis et al. [41] investigated ABM to assess fuel switching and carbon capture and storage in the Chinese ammonia industry. The authors proposed an integrated techno-economic approach for industrial modelling, using ABM implemented within the ModUlar energy systems environment framework. Fundamentally, the proposed ABM framework used a bottom-up methodology for developing energy transition scenarios wherein the model estimated energy consumption, emissions, capital and operating costs for each technology. In the context of renewable energy, Mohammed & Al-Bazi [4] considered an agent-based heuristic optimisation system to manage a comprehensive renewable energy system, including production, storage, distribution, and consumption. A sustainable energy storage strategy was developed using renewable energy surpluses by developing a new heuristic algorithm. This contributed to optimising the energy storage levels in different storage devices to hedge against production descriptions influenced by external uncontrolled factors, such as weather and technical disruptions. This leads to archiving optimised energy storage levels across different located storage devices to face the risk of production shortages due to weather conditions. The developed system was then applied to a case study in Iraq, comprising 12 cities and hybrid renewable energy sources to allow source switching depending on weather conditions, including wind, solar, and hydro. A later study by Yu et al. [42] considered the concept of carbon neutrality for designing, scheduling, optimising, and assessing hybrid renewable energy systems. Using ABM, the proposed framework evaluated scheduling schemes under multi-index systems and analysed the impact of policy parameters on zero-carbon system design.

1.2. Contribution and novelty

In view of the reviewed studies, ABM has gained recognition as a decision-making tool in the context of renewable energy planning and management. However, mathematical programming remains more widely used in designing and planning natural gas infrastructure, as outlined in Table 1. A clear gap exists in applying ABM for the dynamic management of mature natural gas systems or networks. With increasing disruptions in final markets affecting the profitability of existing natural gas projects, ABM emerges as an effective tool for informed decision-making, enabling project performance evaluation under varying market conditions and policies [7]. This work introduces a novel techno-economic ABM approach to optimise annual natural gas allocation strategies for Qatar's established natural gas network. By incorporating variable annual demand and pricing for different commodities, the tool applies upper and lower production limits for each technology, allowing for flexible allocation throughout the planning horizon for enhanced overall project's economic or environmental sustainability.

Given the dynamic nature of natural gas markets, this study assesses the effectiveness of the proposed ABM tool for efficient planning and decision-making within mature natural gas infrastructure. The ABM approach is designed to navigate the complexities of fluctuating market conditions, providing decision-makers with timely insights that enhance the adaptability and resilience of their strategies. Evaluating the tool's performance under various scenarios (4 main cases) demonstrates its potential to optimise planning processes, ensuring more informed and responsive management of natural gas resources.

This study is structured as follows: Section 2 highlights the data and the methodology used to meet the research objective; Section 3 discusses the results of the different investigated cases based on different natural gas network structures under fixed assumptions and input data; Section 4 compares the results of the different cases and highlights the policy

Table 1
A comparison of relevant natural gas infrastructure design and planning studies.

Aspect	Santibanez-Borda et al. [43]	Al-Sobhi et al. [44]	Al-Mohannadi et al. [45]	Current work
Objective	Planning the electrification of hydrocarbon production networks while minimising GHG emissions.	Optimising process design and operations to identify economically and environmentally sustainable pathways for natural gas utilisation.	Designing natural gas utilisation schemes for maximum economic returns while meeting emission limits	optimising natural gas allocation to existing downstream processes based on economic and environmental targets.
Optimisation approach	Multi-objective mixed integer linear programming.	Mixed integer linear programming.	Mixed integer linear programming.	Agent-based modelling.
Planning period	Multi-period	Single period	Single period	Multi-period
Infrastructure considered	Existing infrastructure	Design of new infrastructure	Existing infrastructure	Existing infrastructure
Network considered	Shared power generation between offshore platforms and integrating the networks with wind farms.	Natural gas network: LNG, GTL, methanol production, and various design alternatives for the main processing unit.	Natural gas network: LNG, GTL, cement, aluminium, power, solar photovoltaic, enhanced oil recovery, methanol, etc…	Natural gas network of different power, LNG, GTL, methanol, ammonia, urea and MTBE configurations
Case Study	Real offshore network located in the UK.	Theoretical case study	Theoretical case study	Real methane-based network in Qatar.
Uncertainty	Uncertainty of input parameters by considering upper and lower bounds.	N/A	N/A	Uncertainty on demand and price by varying annual input values.
Policy Implications	Yes	N/A	N/A	Yes

implications; and finally Section 5 summarises the conclusions of the study and the recommendations for future work.

2. Data and methods

The proposed framework in this work utilises technical data (i.e., operational system boundaries and yield rate) along with forecasted demand and prices to optimise annual natural gas allocation to different mature natural gas processes. While the developed ABM approach can be applied to any mature natural gas downstream processes comprising chemical and natural gas monetisation to value-added products, the methodology and input data addressed herein consider Qatar's energy sector, focusing on optimising natural gas utilisation to different products for maximum annual profitability or minimum annual emissions reparented by global warming potential (GWP). Fig. 1 illustrates the overall research framework presented in this work, along with inputs and outputs. For market data, Fig. 2(a) demonstrates historical and forecasted annual demand for natural gas and monetised products between 2000 and 2033 (in million metric tonnes per annum, MMTPA). Fig. 2(b) illustrates the time series of the selling price for each produced product in the period between 2000 and 2033 (in $/tonnes). Fundamentally, all forecasts are extracted from online open-source resources [46–50], wherein interpolation, extrapolation, and GCAR-based techniques are used to estimate missing data points. Additionally, the developed agent-based approach utilises technical (i.e., operational bounds and yield) and cost (i.e., fixed and variable costs) data for each process, estimated using Process Economic Analyzer and Energy Analyzer in Aspen HYSYS.

Subsection 2.1 elaborates on the natural gas downstream processes that are already deployed in Qatar. Subsection 2.2 highlights the components and equations associated with the agent-based model (ABM) to meet the optimisation objective.

2.1. Downstream production systems

The increased pace of demand changes in the final markets induces exploring the impact of annual demand and price variations on managing existing natural gas production portfolios. The state of Qatar, a natural gas-abundant country, utilises natural gas for power generation (i.e., gas to power) to meet the local demand and monetises the surplus to value-added products for targeting international markets. The network incorporates one physical monetisation option, liquified natural gas (LNG), and three chemical monetisation options, gas-to-liquids (GTL), methanol, and ammonia. Additionally, the network considers indirect monetisation of natural gas to products, wherein methanol is used as a feedstock for MTBE production, and ammonia is the primary feed to produce urea. Considering real operational boundaries, the developed ABM tool investigates flexible annual natural gas allocation to the different processes subject to the demand and prices of commodities in international markets. The tool primarily prioritise allocating natural gas to power to satisfy the local demand, while the remaining natural gas capacity is allocated to different processes based on market performance for maximising the annual revenue. Table 2 summarises the lower operational limit for each process in MMTPA, based on data collected from mature technologies deployed in the country.

2.2. ABM simulation

The developed ABM framework predicts portfolio decisions for the downstream natural gas industry in response to rapidly changing market conditions. Economic and environmental scenarios can be analysed when considering natural gas allocation, supported by the operational flexibility of the investigated processes. For the economic scenario, the ABM model aims to allocate natural gas to downstream processes with the objective of maximising the total network's profitability. In contrast, the tool allocates natural gas to the utilisation sinks with the objective of minimising the total emissions in the environmental scenario. The scenario-based assessment allows the decision-maker to investigate different allocation strategies based on the required target (i.e., economic or environmental) to evaluate potential trade-offs.

In ABM, the model comprises a group of agents, with a set of characteristics and behaviours, interacting within an environment to meet a target subject to rules (i.e., constraints) [51]. In this analysis, two main groups of agents are considered for the allocation of direct and indirect natural gas to different downstream processes (i.e., power, LNG, GTL, ammonia, methanol, urea, and MTBE), adhering to technical limitations to achieve economic or environmental objectives. This ABM model simulates energy sector selections over a 34-year period (N=34), with natural gas generating systems NG serving as the primary agent. The primary agent interacts with a secondary agent represented by $Di, Di \in D$, where D is the set of downstream processes. Both groups of agents interact within an environment that is influenced by domestic and global economies. Table 3 summarises the characteristics of each group of agents. Fig. 3 represents the ABM elements, including agent groups, the environment, and the type of interaction between the group of agents.

2.2.1. Agents

The presented model comprises two main groups of agents: the

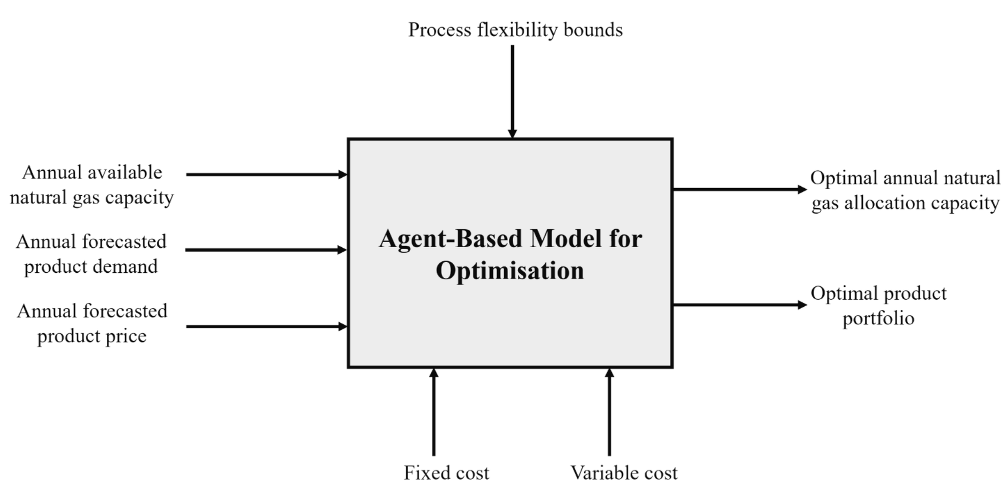

Fig. 1. Overall framework for optimising annual natural gas allocation to process routes.

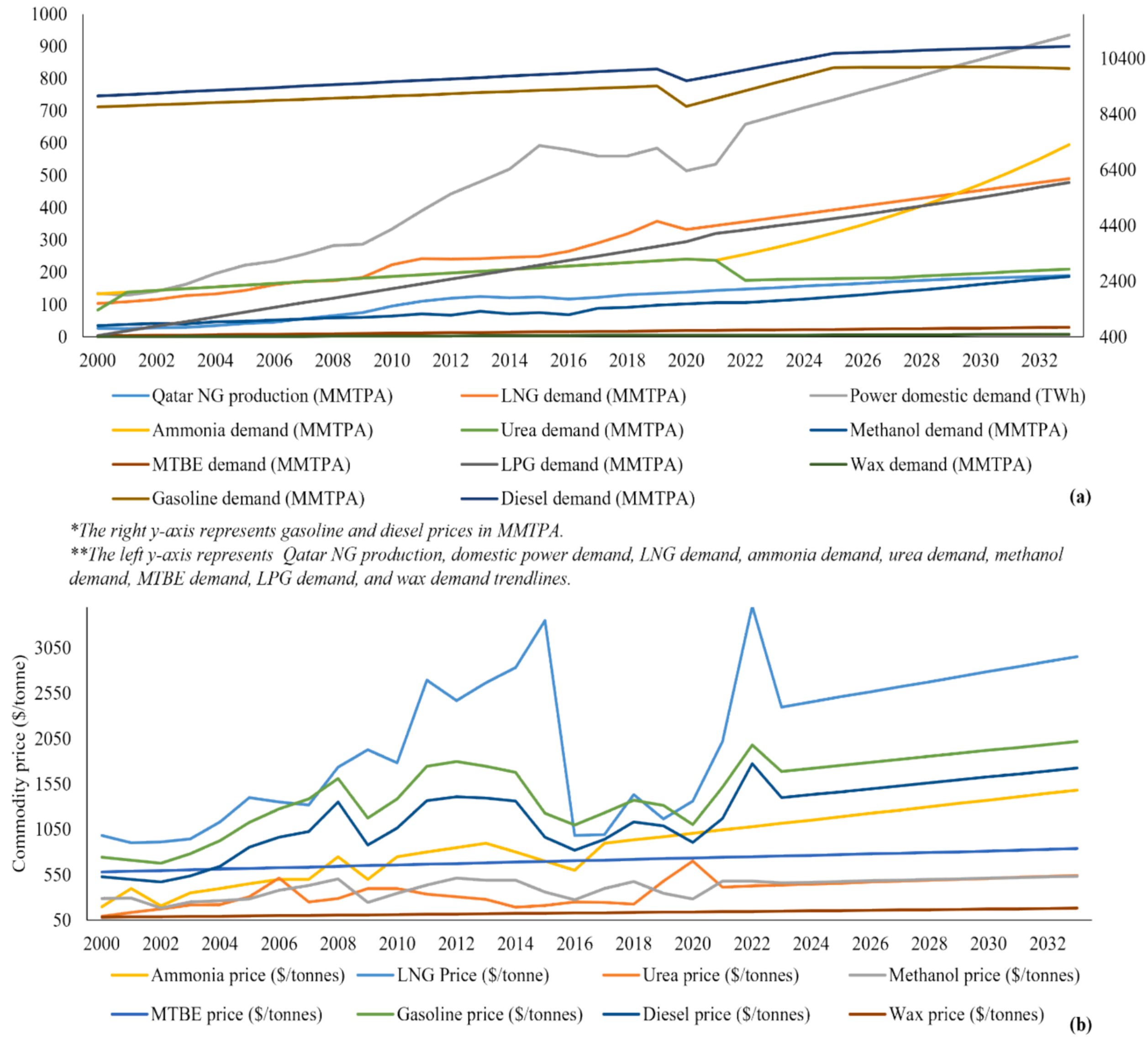

Fig. 2. Input market data used for optimising natural gas allocation; (a) market demand and (b) price for each commodity.

Table 2
Lower operational flexibility bounds for the considered processes.

Process	LNG	Fischer-Tropsch GTL				Methanol	MTBE	Ammonia	Urea
		LPG	Diesel	Gasoline	wax				
Minimum production (MMTPA)	5	0.012	2.41	0.76	0.57	0.83	0.61	3.8	5.6

natural gas system (*NG*), and the downstream industries system (*Di*). Each agent has a unique strategy to satisfy the overall allocation target.

A. Agent Group (1): Natural gas system (NG)

The NG system is the central element of the model as it ensures the yearly allocation of the available capacity of natural gas (*Cng*) to four downstream industries (i.e., sinks): power, LNG, MTBE, methanol, GTL, ammonia, and urea. The allocation strategy to sinks is accomplished based on two strategies: (1) to meet the local demand for power (*p*) or (2) to optimise the allocation to LNG (*l*), GTL (*g*), Ammonia (*a*), Urea (*u*), Methanol (*m*), and MTBE (*b*) in alignment with the global demand. The allocation decision is influenced by environmental factors (i.e., emissions), economic factors (i.e., profitability and demand), and operational characteristics (i.e., yield and production capacity). Fig. 4 illustrates a roadmap of the behaviour taken by the *NG* system to meet the NG allocation target.

B. Agent Group (2): Downstream processes system (Di)

In this analysis, the NG system first satisfies the local power demand before allocating the surplus natural gas capacity to 6 direct and indirect sinks, regarded as *Di*. The ideal allocation strategy to the 6 sinks (i.e., LNG, GTL, methanol, MTBE, ammonia, and urea) is determined based on the yearly operational production capacity of each sink (*Ci*), the domestic power demand (*Pi*), and the minimum flexible production for each sink (*Dmin*). Fig. 5 demonstrates a roadmap for the behaviour taken by the *Di* system for decision-making.

Economic (EC) and environmental indicators (EI) were used to analyse the performance of both agent groups, *Di* and *NG*. Equations (1–2) are used at each time step, $n \in N$, to estimate the EC and EI for strategy (*NG*). While Equations (3–4) are considered for estimating the indicators for strategy (*Di*).

Table 3
Attributes and Behaviours associated with agents,

Agent	Attributes	Behaviours
NG system (*NG*)	– Total NG capacity *C* (Billion cubic meters, BCM). – Annual NG distribution capacities *Cng* (BCM) – Annual NG allocation to Power *Qp*, LNG *Qn*, GTL *Qg*, Ammonia *Qa*, Urea *Qu*, Methanol *Qm*, and MTBE *Qb* – Global Warming Potential (GWP) from generating each product (tonnes of CO_2eq)	– Allocate NG to Power *(p)*, LNG (*l*), GTL (g), Ammonia (*a*), Urea (*u*), Methanol *(m)*, and MTBE *(b)*.
Downstream Processes (*Di*)	– Annual production capacities Q_{Di} (kg) – Annual power local demand *Pi* (kWh)	– Determine the best production sinks (*S*).

$$EC_{NG} = Q_{i,NG} \times c_{i,NG} \quad (1)$$

$$EI_{NG} = Q_{i,NG} \times e_{i,NG} \quad (2)$$

$$EC_{D} = Q_{i,D} \times c_{i,D} \quad (3)$$

$$EI_{D} = Q_{i,D} \times e_{i,D} \quad (4)$$

Where $Q_{i,NG}$ is the annual natural gas allocation to process *i* (in BCM), and $c_{i,NG}$ is the net cost for natural gas allocation to process *i* (in \$/BCM) simulated using Aspen HYSYS Economic Analyzer. Process *i* is *p* (power), *l* (LNG), *g* (GTL), *a* (Ammonia), *u* (Urea), *m* (Methanol), and *b* (MTBE). For Equation (2), $e_{i,NG}$ measures the environmental impact, estimated as the global warming potential (GWP) by the Energy Analyzer in Aspen HYSYS for natural gas allocation to process *i*. Similarly, $Q_{i,D}$ in Equation (3) & (4) is the annually produced products from process *i* (in MMTPA) or (in kWh) for power. $c_{i,D}$ is the revenue for product sales (in \$/MT) for products or (\$/kWh) for power. While $e_{i,D}$ is the GWP associated with product generation from process *i*. Overall, the values estimated by equations (1)-(4) are determined by ABM decisions that are subject to available natural gas capacity, domestic power demand, global market

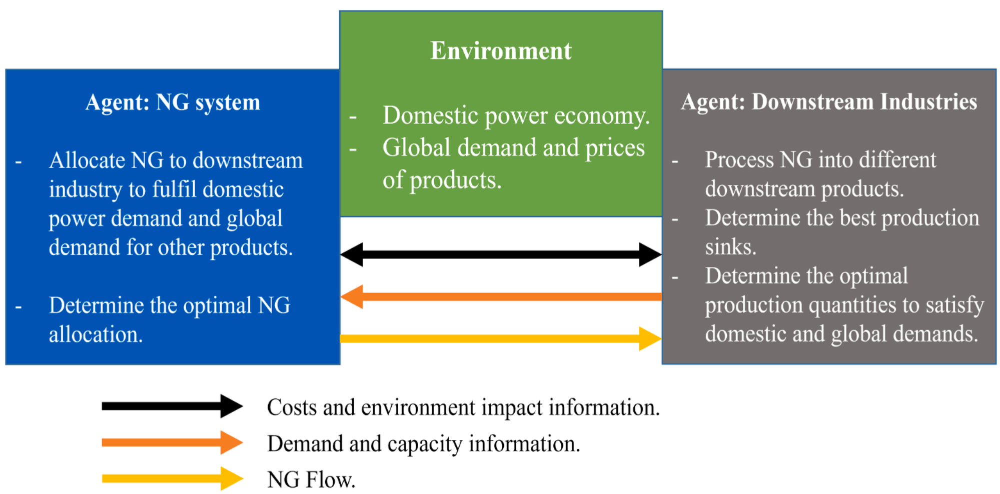

Fig. 3. A demonstration of the different elements involved in the ABM.

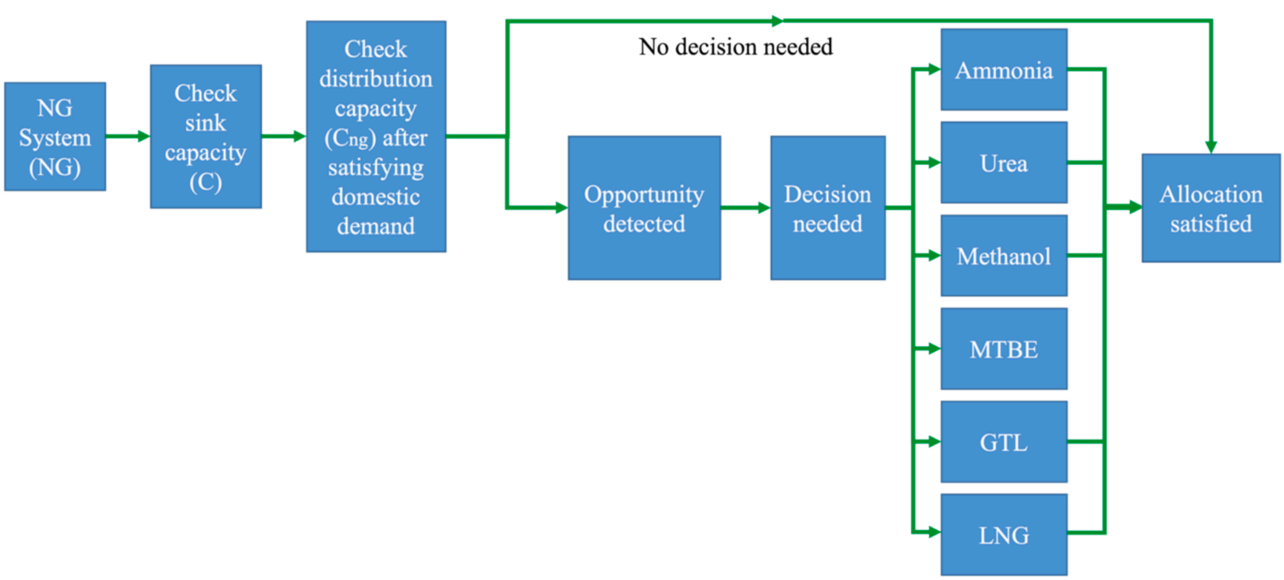

Fig. 4. Demonstration of the *NG* system agent behaviour for decision-making.

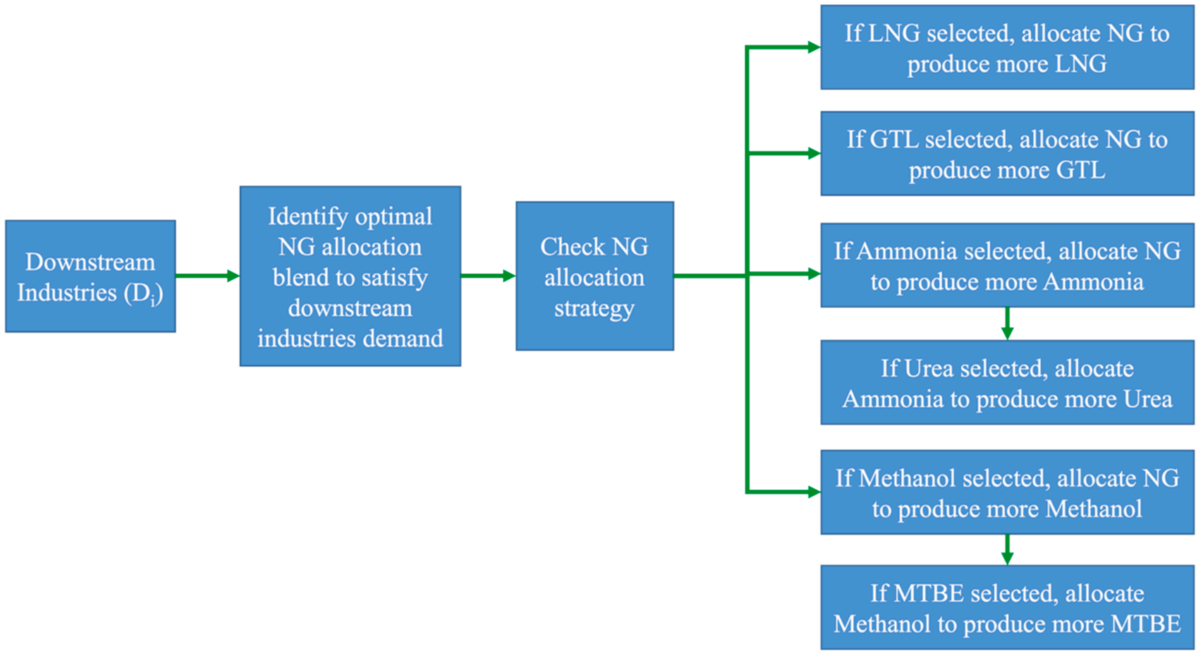

Fig. 5. Demonstration of the downstream industries' (*Di*) agent behaviour for decision-making.

performance, and flexibility constraints for each process.

Using the Python-based MESA library in Google Collaboratory Notebook, the ABM approach was investigated for the system under several case studies, as discussed in section 3. Fundamentally, MESA supports the rapid generation of agent-based models, utilising pre-built essential components, such as spatial grids and agent schedulers or personalised implementations. A sample code for case A has been provided in the supplementary materials.

3. Results and discussion

Agent-based modelling is identified as essential for managing natural gas export portfolios by simulating complex interactions among various agents. The dynamic approach models market conditions, pricing strategies, and geopolitical influences, considering factors, such as demand fluctuations, supply chain disruptions, and regulatory changes. This, in turn, allows decision-makers to assess resilience, identify vulnerabilities, and make informed decisions to enhance the overall robustness of natural gas export management. Considering technical data and forecasted market trends, this study employed ABM to determine the optimal allocation of natural gas to industrially mature downstream industries in Qatar under economic and environmental scenarios. Typically, LNG facilities in Qatar receive the highest allocation, although the results presented herein explore flexible allocations based on different network configurations. Inspired by the "real options" theory, the economic strategy adjusts allocations to maximise profitability, allowing increasing production during bullish markets and reducing production as a risk-hedging strategy during bearish market conditions. Meanwhile, the environmentally-driven strategy aims to minimise the overall emissions regardless of economic factors. The findings indicate that the allocation strategy significantly impacts agent behaviour, influenced by changing annual capacities and fluctuating demands and prices.

The results presented herein are divided into four main subsections, each highlighting a distinct case study under economic and environmental scenarios. Section 3.1 elucidates the outcomes of monetising natural gas into power generation, LNG, ammonia, and urea (case 1). Section 3.2 delves into the results of converting natural gas into hydrogen-based commodities, focusing on the cost-effectiveness and environmental implications of the routes (case 2). Section 3.3 describes the results of an integrated network approach, encompassing the production of LNG, ammonia, methanol, urea, GTL, and MTBE, highlighting synergies and trade-offs within the network (case 3). Finally, Section 3.4 synthesises the findings from the overall monetisation network and power generation to provide a holistic view of the economic and environmental performance (case 4). While the first two cases prioritise the production of high-demand commodities (i.e., LNG and hydrogen carriers), the latter two highlight the economic and environmental sustainability of operating Qatar's existing natural gas (i.e., methane-based) network with greater flexibility. Additionally, the natural gas to power route is excluded in cases 2 and 3 to assess the economic and environmental sustainability of dedicating natural gas for export purposes. Overall, case 4 reflects the current network in practice, while other cases aid with policy and investment decision-making.

3.1. Case 1: Natural gas to power, LNG, ammonia, and urea

Supported by the bullish potential of ammonia and urea as hydrogen storage media, the first case utilises ABM for optimising the allocation of natural gas to power, LNG, ammonia, and urea, evaluated for the period between 2000–2033 under varied annual demand and price data [52–54]. The NG allocation system recommends a poly allocation strategy under the economic scenario to meet local power demands and international downstream product demands, as illustrated in Fig. 6 (a). As demonstrated in the figure, the economic factor drives the highest proportion of natural gas to LNG, followed by ammonia in some years (i.e. 2017, 2019, and 2020) for part of the energy mix. On the contrary, under the environmental scenario, the NG allocation strategy prioritised ammonia over LNG throughout the planning horizon (Fig. 6(b)) after prioritising meeting domestic power requirements. Compared with the economic scenario, the decline in the allocated share to LNG is attributed to the significant emissions associated with the liquefaction process. In turn, the dominance of ammonia as a cleaner utilisation route increases the share of urea production. Fig. 7 (a-b) illustrates the annual net profit (in million \$/y) and annual emissions (in million CO_2eq t/y) estimated for NG allocation under economic and environmental scenarios. Fundamentally, an environmental-based allocation strategy allows the producer to reduce the GWP emissions by an average value of 4% compared to the economic approach. However, an increase of 55%

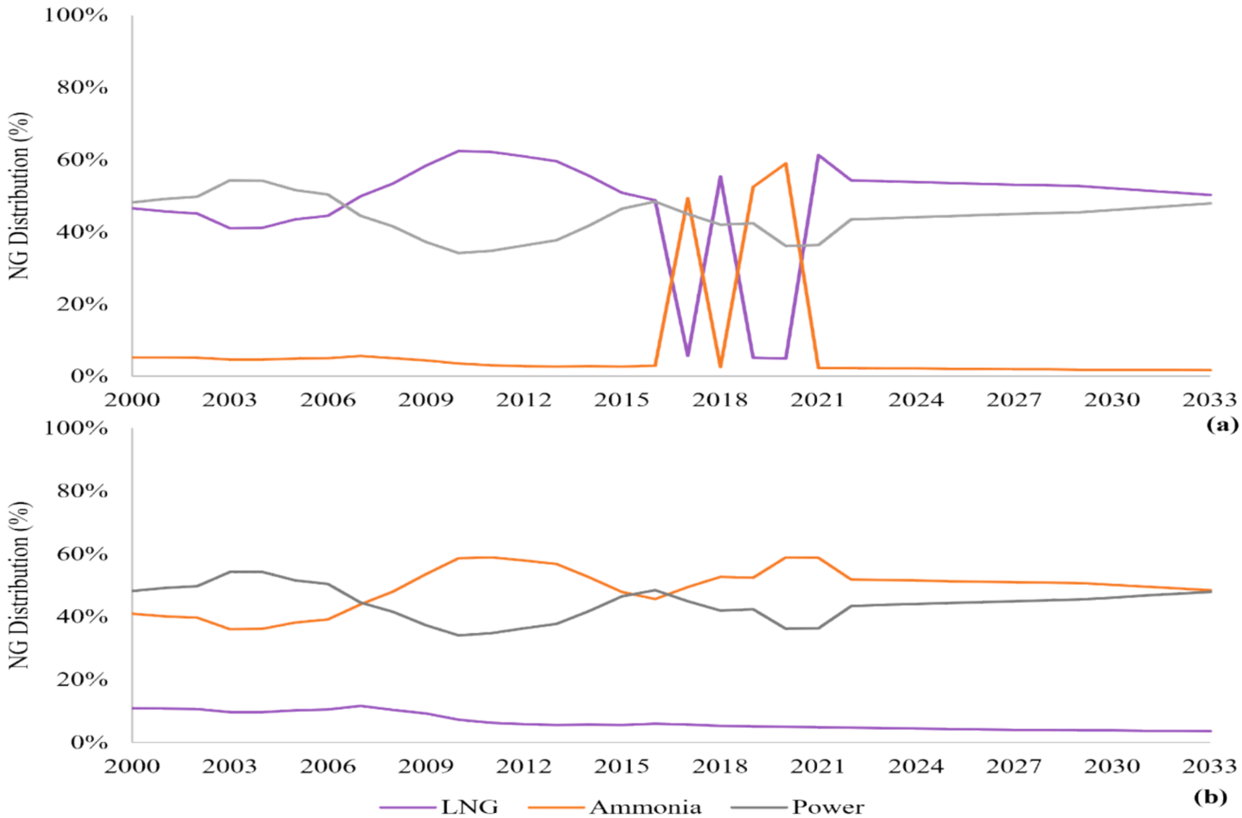

Fig. 6. Annual share of natural gas allocated to direct processes (i.e., LNG, ammonia, and power) under (a) economic and (b) environmental scenarios.

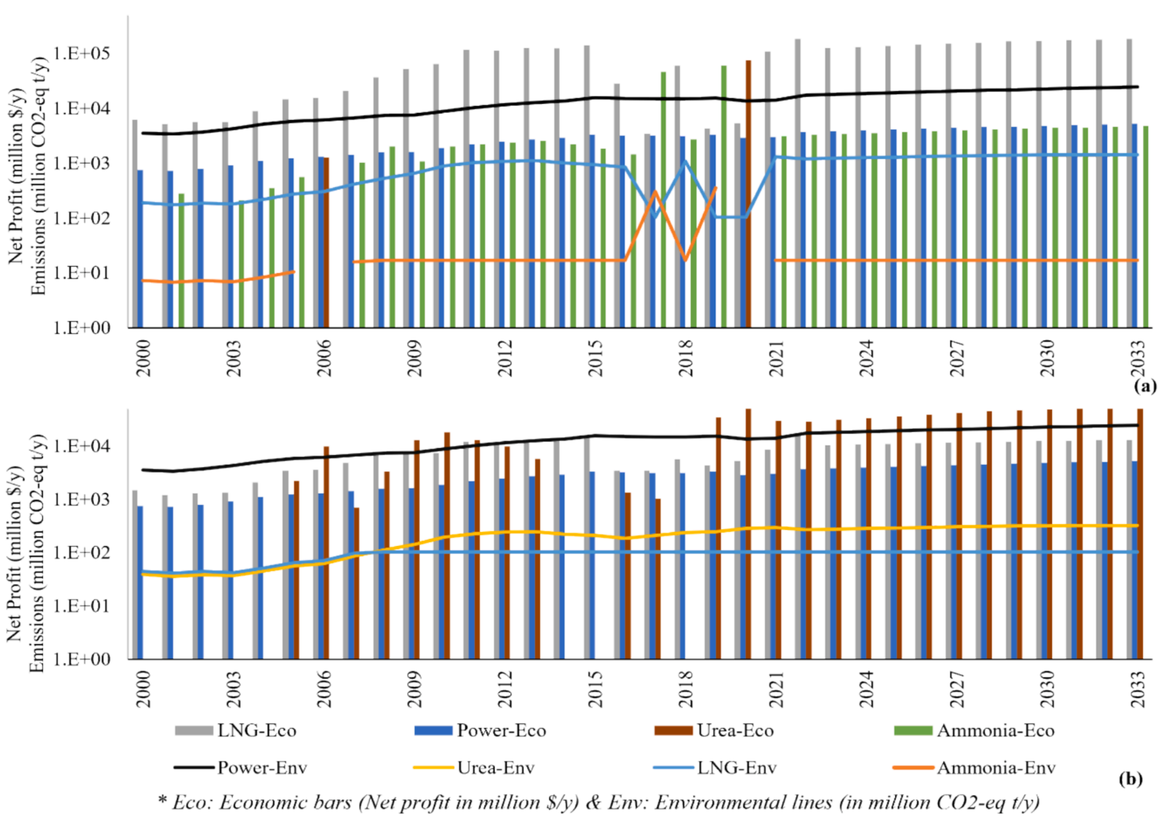

Fig. 7. Annual profitability and emissions associated with the natural gas allocation to LNG, power, ammonia, and urea, based on (a) economic and (b) environmental scenarios.

in costs associated with infrastructure deployment and operating costs is be needed to meet the 4% reduction in emissions.

3.2. Case 2: Natural gas to hydrogen-based routes

With increased interest in cleaner energy resources, a shift to hydrogen has been identified due to its versatility and environmental sustainability as an energy carrier. The second case presented herein evaluates the economic and environmental attractiveness of allocating the produced natural gas capacity to hydrogen-rich routes for export purposes. Under the economic scenario, the model prioritised allocating more than 80% of the available NG capacity to the GTL process to produce LPG, diesel, gasoline, and wax in the period between 2000–2014 (Fig. 8 (a)). On the contrary, the allocation strategy significantly shifted to prioritising ammonia from 2015 until the end of the planning horizon. Fundamentally, the shift to ammonia could be attributed to changes in market dynamics, including prices and demand, and the increased interest in cleaner fuels driven by policy and regulatory drivers. Interestingly, the high emissions associated with the GTL and ammonia processes have diverted the model to shift to methanol as a utilisation route from 2007 until the end of the planning horizon, as illustrated in Fig. 8(b). The increased production of methanol, in turn, allows for an additional production capacity of MTBE compared to the economically driven scenario, as illustrated in Fig. 9(a-b). The environmental-based allocation results in an average decline in annual profitability of 20% and an average annual GWP reduction of 33% compared to the economic scenario.

3.3. Case 3: Full network

From another perspective, investigating the model's behaviour subject to changing market dynamics (i.e., the change in the demand for conventional and cleaner fuels) is crucial for informed decision-making. In this case, the model investigates optimal NG allocated share to a methane-based network comprising liquefaction, ammonia, methanol, GTL direct processes, and MTBE, and urea in-direct processes. The full production of natural gas capacity is assumed to be dedicated to exporting to international markets, wherein power demand is assumed to be covered using alternative energy resources, such as solar panels. As illustrated in Fig. 10 (a-b), natural gas allocation to the liquefaction process for LNG production dominated both strategies. Fundamentally, the period between 2017 and 2020 witnessed a disturbance in the market that influenced the model's decision towards prioritising liquefaction as per the economic allocation scenario. This could be attributed to the increase in global LNG supply pumped into the market by competitors, including the US and Australia. Additionally, the decline in the global energy demand in 2020 and increased demand for agricultural fertiliser was a driving factor towards prioritising ammonia production. The decline trend towards GTL is observed to be dominant in both allocation scenarios. This is attributed to the high fixed and operating costs in the economic scenario. In the environmental scenario, the significant GWP associated with the GTL process constrained the share of allocated natural gas to the GTL route (Fig. 11(a-b)). Prioritising LNG as a monetisation route in both scenarios, in turn, resulted in the highest revenue amongst the several utilisation routes, with an average profitability of \$131 billion and \$135 billion for the economic and environmental scenarios, respectively. The prioritisation of LNG in both strategies did not impact the estimated emissions, with an emission reduction of almost 0%. The analysis reveals minimal trade-offs between the two scenarios presented in this case, offering critical insights into the potential for transitioning to cleaner energy resources for power generation for reducing emissions within the sector.

3.4. Case 4: Full network with power

In a business-as-usual scenario, the State of Qatar utilises natural gas for power generation to meet the needs of households and commercial sectors. This case prioritises meeting the demand requirement of power, wherein the surplus natural gas is allocated to the different chemical and physical monetisation routes for international export. Regardless of the allocation restrictions (i.e., economic or environmental), the ABM prioritises allocating natural gas to meet the total power requirement. Hence, as illustrated in Fig. 12(a-b), the trend and annual values of the natural gas share allocated to power are fixed. In contrast, both

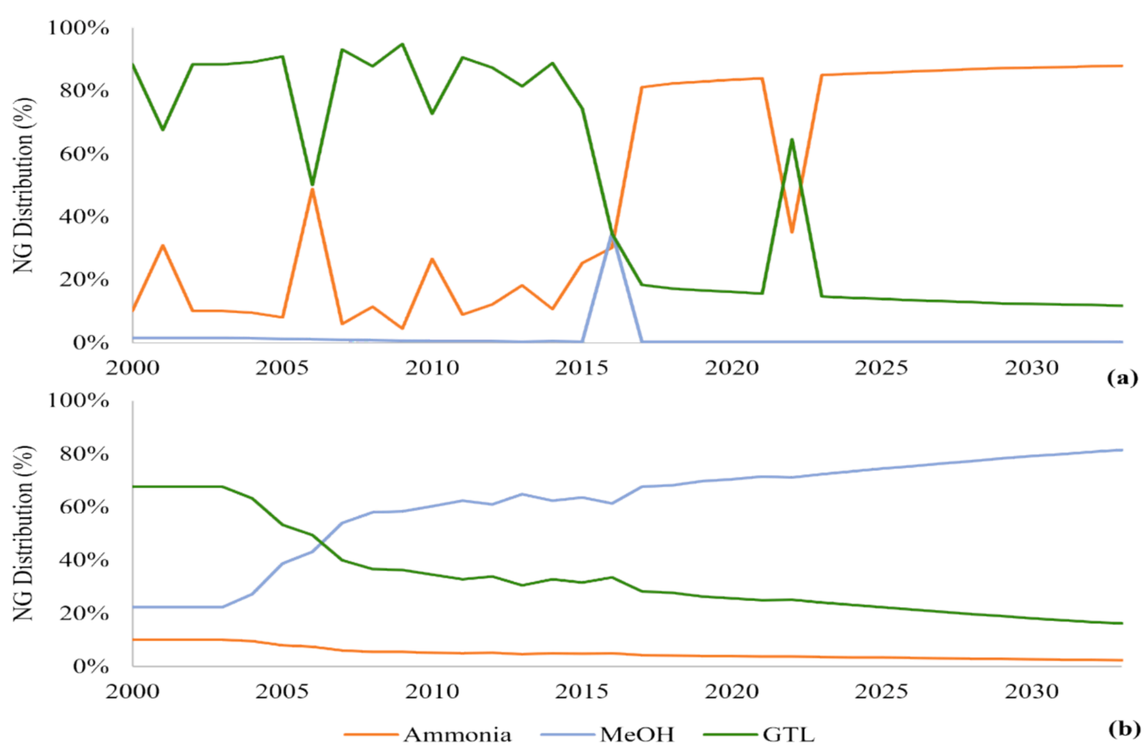

Fig. 8. Annual share of natural gas allocated to hydrogen-rich direct processes under (a) economic and (b) environmental scenarios.

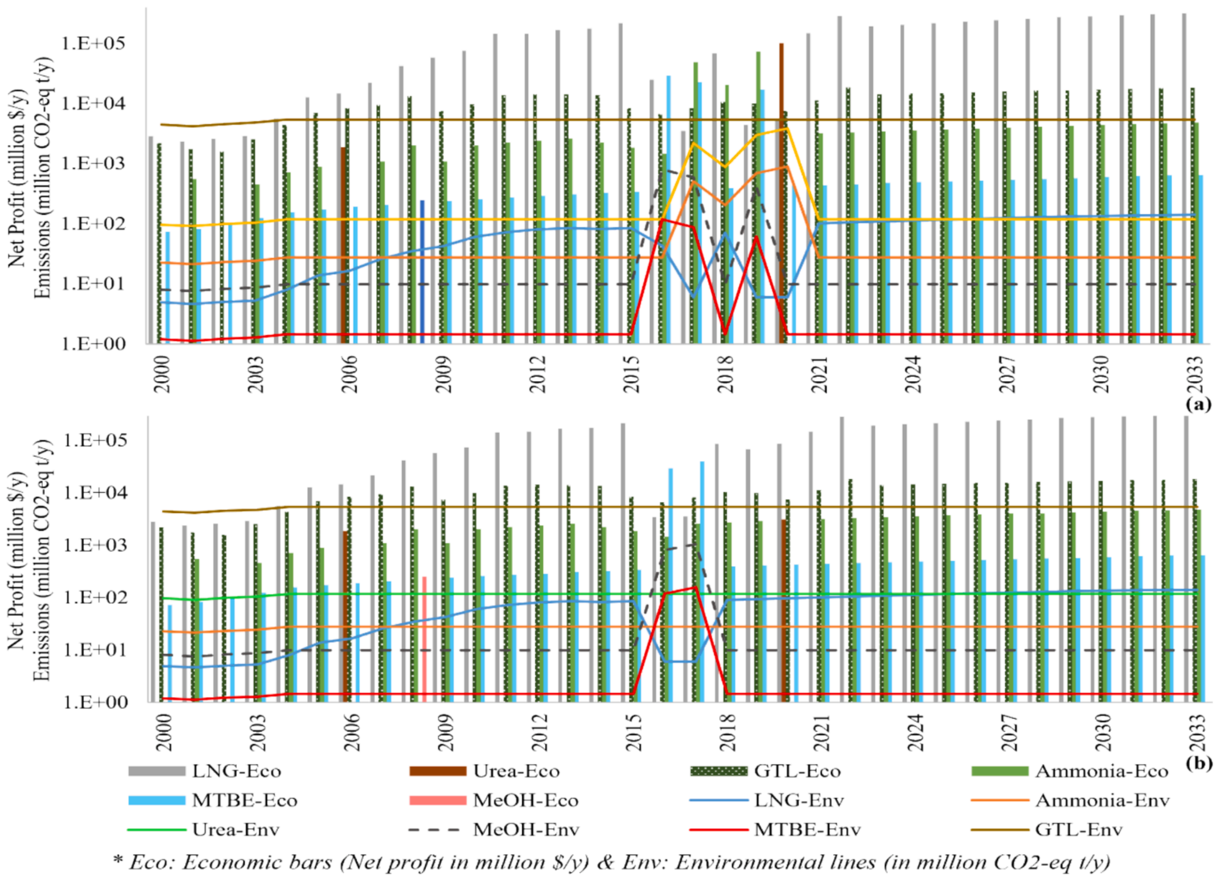

Fig. 9. Annual profitability and emissions associated with the natural gas allocation to hydrogen-rich processes and their derivatives, based on (a) economic and (b) environmental scenarios.

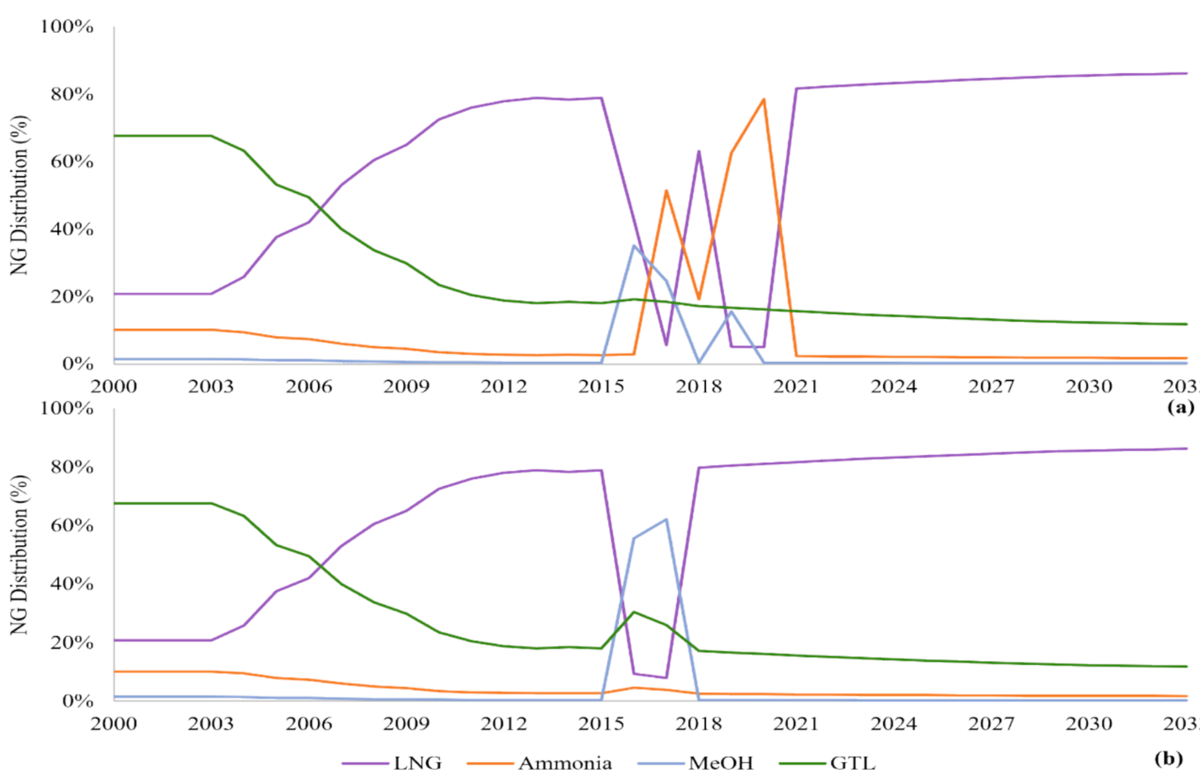

Fig. 10. Annual share of natural gas allocated to direct processes in the full network under (a) economic and (b) environmental scenarios.

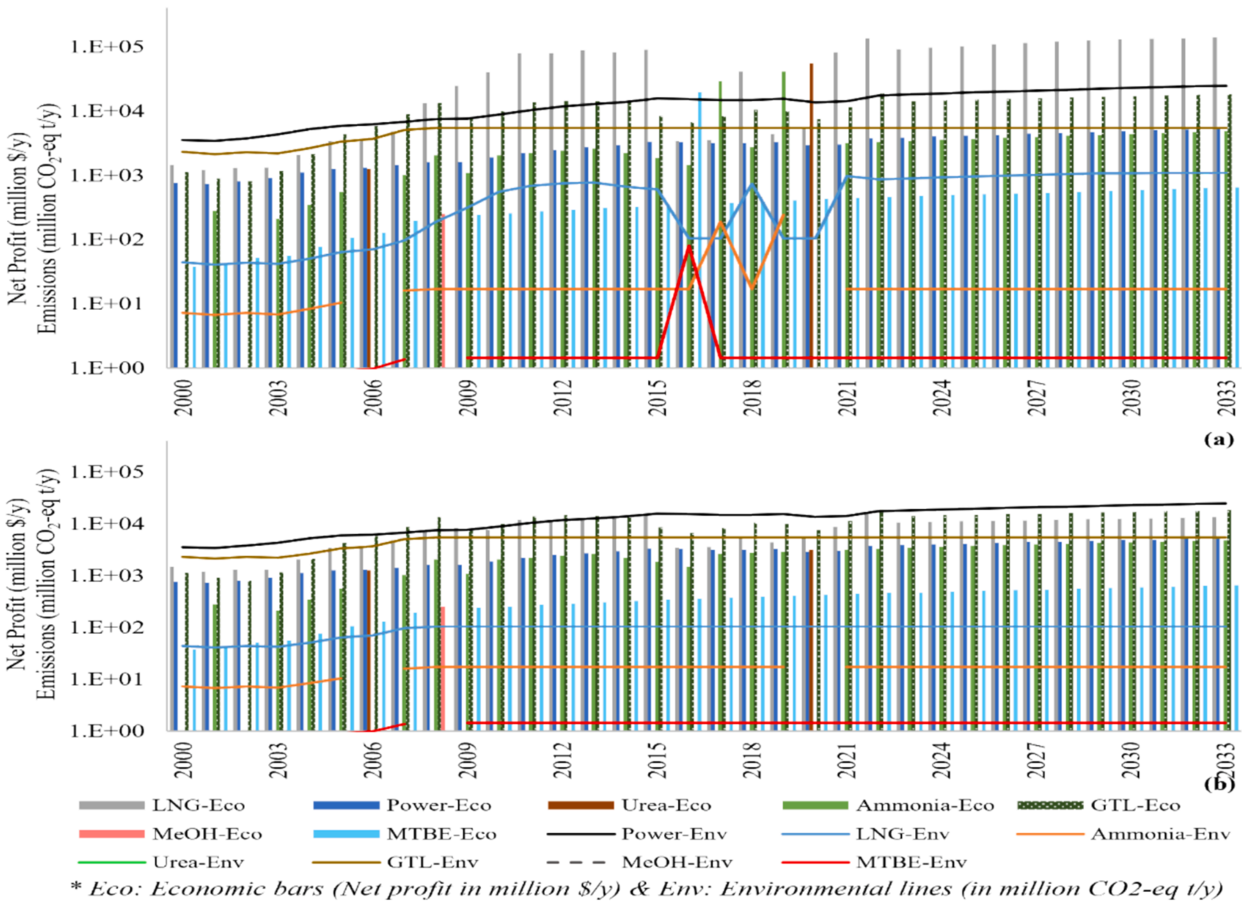

Fig. 11. Annual profitability and emissions associated with the natural gas allocation to processes of the full network and their derivatives based on (a) economic and (b) environmental scenarios.

allocation strategies resulted in the same natural gas allocation trend to the GTL process due to the lower bound constraint that pushes the tool to meet the minimum operational requirement. The investigation revealed a discernible variance in tool allocation behaviour between the liquefaction, ammonia and methanol processes. The economic factor emerged as the primary catalyst for heightened turbulence in the economic allocation strategy, notably from 2015 to 2021. This turbulence was principally induced by significant market perturbations, including the oil crisis and the COVID-19 pandemic. These disruptive events exerted considerable influence on the allocation dynamics, amplifying the complexity of decision-making processes within the specified timeframe. After this timeframe, the escalation of natural gas prices incentivised the model to prioritise LNG production. On the contrary, the environmental allocation strategy prioritised LNG production over ammonia and methanol (Fig. 12(b)) throughout the investigated planning horizon to meet the requirement of minimising emissions while maintaining the production at least at the lower operational bound of each process. Fundamentally, while LNG and GTL products are sold directly to markets, the ammonia and methanol produced through direct natural gas utilisation are used in subsequent processes to produce urea and MTBE, respectively. Fig. 13(a-b) illustrates the profitability and emissions associated with each allocation strategy. It is evident that the emissions attributed to power generation exert a dominant influence in both investigated cases. Meanwhile, in terms of profitability, LNG and GTL represent noticeably high profitability margins. Furthermore, the findings indicate that a significant proportion of the produced methanol was directed towards the production of MTBE. At the same time, the ammonia-to-urea route was prioritised solely in the years 2006 and 2020 across both economic and environmental scenarios. Overall, the significance of the restriction to meet power demand in both strategies allowed the model to mitigate greenhouse gas emissions by an average value of only 2%. Yet, it reduced the annual profitability by an average value of 69%. The decision-maker is tasked with navigating trade-offs inherent in considering both economic and environmental scenarios, highlighting the imperative to reconcile competing priorities and optimise outcomes across these divergent domains.

4. Case comparison and policy implications

The cases investigated in this study focuses on optimising natural gas allocation for various network configurations at fixed input parameters under economic and environmental scenarios. Overall, it is observed that cases excluding meeting the domestic power requirement achieved higher profitability and fewer total emissions compared to the cases that obliged the model to prioritise the domestic power demand prior to allocating the surplus natural gas to downstream processes. The four analysed cases are scrutinised to assess their effects on network profitability and emissions. Case 1 is tailored to address power requirements, resulting in diminished profitability and reduced emissions relative to case 2 (i.e., hydrogen-rich utilisation routes). Cases 3 and 4 share identical network configurations yet diverge in power requirements. Specifically, case 3 incorporates power requirements, whereas case 4 does not. Table 4 and 5 summarise the optimised total profitability (in billion $) and/or total emissions (in billion CO_2eq tonnes) under economic and environmental scenarios for the overall historical and forecasted studied period. The analysis is conducted separately for two distinct periods: 2000–2023 (historical) and 2024–2033 (forecasted). The historical period represents what could have been the optimal

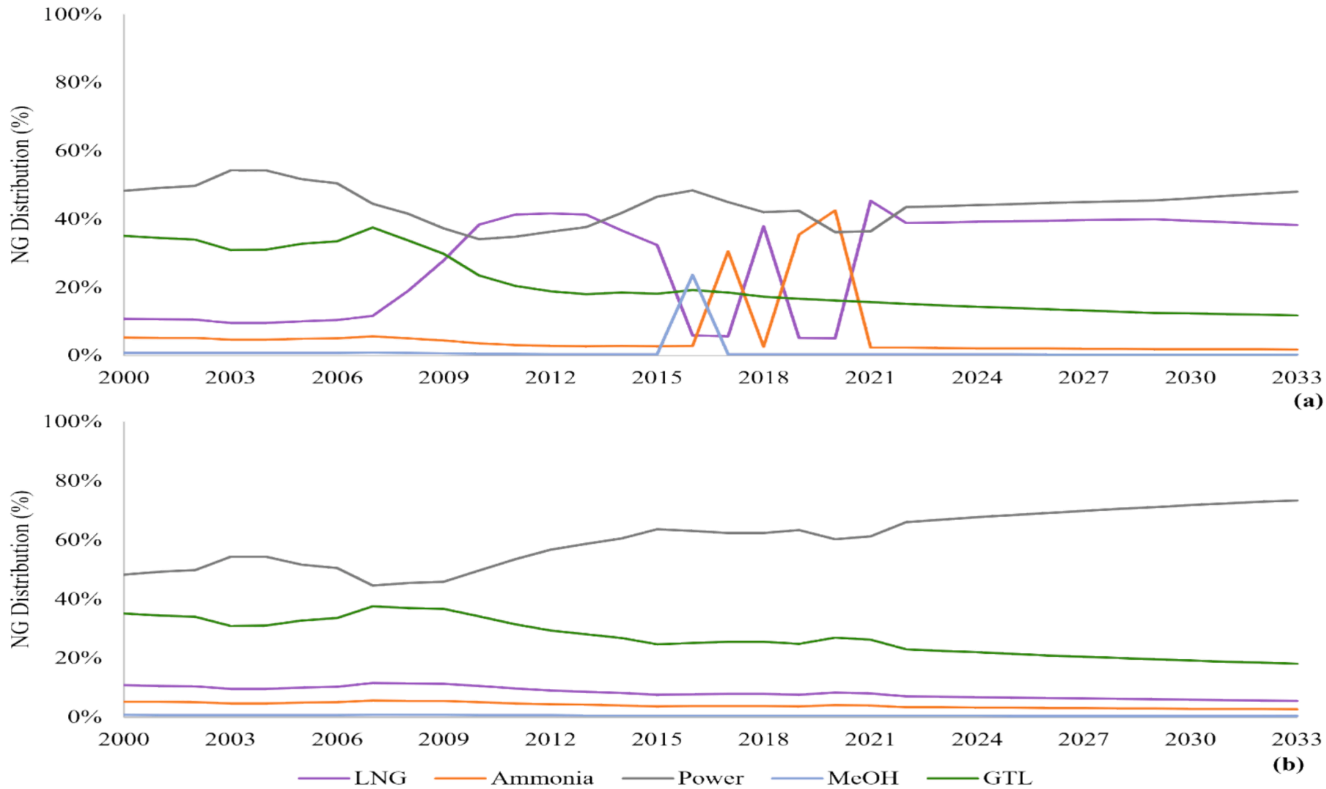

Fig. 12. Annual share of natural gas allocated to direct processes in the full network with power under (a) economic and (b) environmental scenarios.

allocation under flexible operations, benefiting from accurate, real-world market data. In contrast, the forecasted period relies on projected values, which are inherently subject to uncertainty and volatility. This separation allows for a clear distinction between the reliability of past data and the potential variability of future scenarios.

For the optimisation based on historical data (Table 4), case 2 represented 4.3% greater profitability than case 1 under the economic scenario when focusing on hydrogen-rich routes and excluding power requirements. This, in turn, contributed to an increase in the total emissions by 40%. Case 2 exhibited 26% more emissions and 49% greater profitability than case 1 for the same cases under the environmental scenario. On the contrary, case 3 achieved 47% more profitability and 2% less emission than case 4 under the economic scenario, while optimising the cases under the environmental scenario represented a higher profitability of 40% and fewer emissions by 3% of case 4 compared to case 3. Hence, with a slight difference in emissions reduction when optimising under the environmental scenario, a decision-maker shall consider the trade-offs between the economic and environmental factors when moving from the quantitative assessment phase to the implementation phase. Overall, case 3 represented the highest profitability when optimising under the economic scenario, while case 1 exhibited the lowest emissions under both economic and environmental optimisation scenarios. Interestingly, considering power in case 1 resulted in enhanced profitability compared to the network configuration considering methanol, GTL and MTBE in case 4 (economic scenario). This could be attributed to the restrictions imposed by the operational constraints to meet the lower operational bound of all processes before allocating surplus natural gas to profitable processes. Hence, satisfying the lower operational bounds of each process reduces the available natural gas capacity for allocation to the more profitable utilisation route, the ammonia process.

With a focus on the future market between 2024 and 2033, Table 5 summarises the optimised total profitability and/or emissions under economic and environmental scenarios using forecasted market data as input data. Overall, the forecasted cases exhibited similar trends to the historical cases for the planning period between 2000–2023. Yet, case 3 demonstrated similar optimised and calculated values based on economic and environmental scenarios wherein a total profit value of $2830 billion and an emissions value of 275 billion CO_2eq tonnes are estimated under different allocation targets (economic and environmental). This, in turn, reflects the resilience of the considered network for the planning horizon (2024–2033) when considering fixed input data and varied allocation objectives. As demonstrated in Table 5, although case 3 exhibited higher profitability than case 4 under the economic scenario (i.e., case 3 total profit of $2830 billion compared to case 4 total profit of $1580 billion), the associated emissions value under the economic scenario of case 4 was higher than case 3 (i.e., case 3 value of 275 billion CO_2eq tonnes compared to case 4 value of 283 billion CO_2eq tonnes). A slight difference of 0.4% between the optimised emission values of the two cases is noticed when optimising under the environmental scenario.

Overall, compared to the economically driven allocation, environmentally driven decision-making exhibited more static allocation strategies throughout the planning horizon due to data limitations. With the objective of minimising total emissions associated with natural gas processing, the tool allocates natural gas to sinks with the objective of emissions reduction regardless of global market demand and prices. A more dynamic annual allocation trend is anticipated when introducing policies and emissions mitigation regulations as input data to be met by producers annually. Hence, the ABM tool could be valuable in assessing decision-makers with prompt outcomes by simulating several cases using different constraints, input data, and optimisation objectives. This includes considering different combinations of renewable share for power generation or multiple CO_2 emissions targets as constraints.

In the literature, Okonkwo et al. [55] investigated Qatar's grid integration of renewable resources (i.e., wind, solar, and biomass) and storage systems. The authors stated that the biggest obstacle to a 100% renewable energy scenario in the country is related to storage. Hence, a decision-maker can investigate integrating technically validated cases given by other studies with investigated scenarios in this work to assess

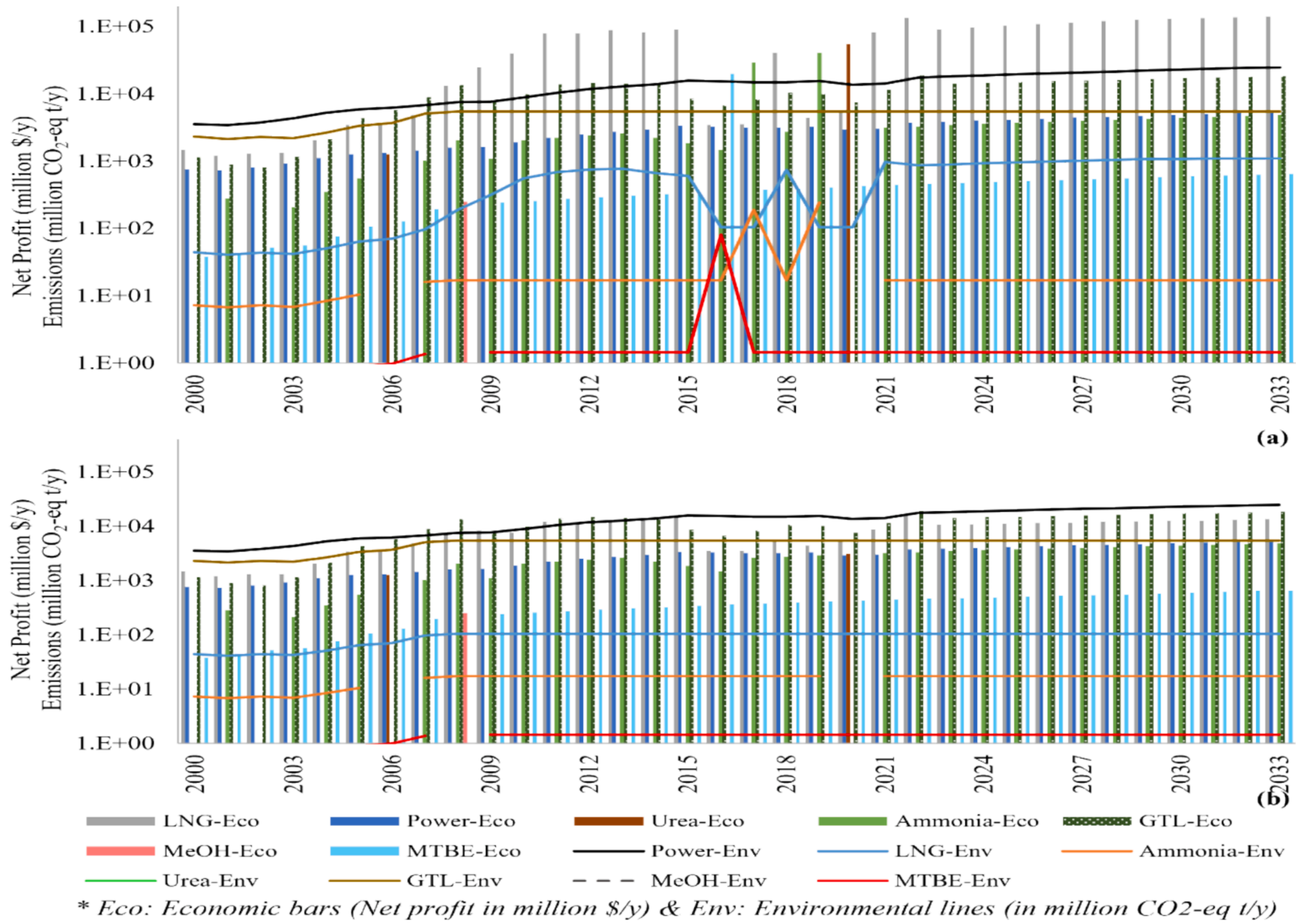

Fig. 13. Annual profitability and emissions associated with the natural gas allocation to processes of the full network with power and their derivatives based on (a) economic and (b) environmental scenarios.

Table 4
Total optimised profitability and/or emissions for the four cases under economic and environmental scenarios for the 33-year planning horizon (2000–2023).

		Case 1	Case 2	Case 3	Case 4
Economic scenario	**Total profit (bn $)**	3.35 x 10^3	3.5 x 10^3	5.22 x 10^3	2.79 x 10^3
	Total emissions (bn CO_2eq t)	5.00 x 10^2	8.30 x 10^2	6.69 x 10^2	6.55 x 10^2
Environm scenario	**Total profit (bn $)**	1.10 x 10^3	2.14 x 10^3	5.13 x 10^3	8.52 x 10^2
	Total emissions (bn CO_2eq t)	4.80 x 10^2	6.57 x 10^2	6.59 x 10^2	6.38 x 10^2

Table 5
Total optimised profitability and/or emissions for the four cases under economic and environmental scenarios for the 10-year planning horizon (2024–2033).

		Case 1	Case 2	Case 3	Case 4
Economic scenario	**Total profit (bn $)**	1.70 x 10^3	2.09 x 10^3	2.83 x 10^3	1.58 x 10^3
	Total emissions (bn CO_2eq t)	2.32 x 10^2	2.80 x 10^2	2.75 x 10^2	2.83 x 10^2
Environm scenario	**Total profit (bn $)**	6.25 x 10^2	1.26 x 10^3	2.83 x 10^3	3.79 x 10^2
	Total emissions (bn CO_2eq t)	2.22x 10^2	2.75 x 10^2	2.75 x 10^2	2.74 x 10^2

the optimal allocation strategies under economic and environmental scenarios. In such integrated scenarios, different shares of renewable power generation can be investigated for different natural gas network configurations. Based on simulation assessments, the scenarios would address the requirements for renewable energy and the associated emissions. For example, a simulated 11 TWh of electricity production, accounting for 23.4% of electricity demand and yielding 19.34 million tonnes of emissions, represents a 21% reduction in emissions compared to the full reliance on natural gas for power generation.

The results of the ABM-based scenarios demonstrate the added value of operational flexibility throughout a project's lifetime wherein a natural gas network is more responsive to the changing market conditions (i.e., global demand and prices) or local and/or international climate policies. The operational flexibility would allow a producer to position itself in the market by capturing high market opportunities when the demand is high and risk against risks when the demand is low. The dynamic annual operations result in a varied annual production portfolio that is optimised based on market performance, available resources, technical constraints, and emissions regulations. Yet, a decision-maker must consider long-term contractual obligations with customers when assessing dynamic operations. From another perspective, while no strict emissions regulations are currently alarming the natural gas industry in Qatar, a prompt understanding of future potential emission taxes (i.e., CO_2 tax) on the estimated profitability will allow producers to decide on an optimal allocation strategy to hedge against emissions-associated risks. Additionally, the tool can be extended to strategise the optimal integration of carbon capture utilisation and storage technologies within the system to provide decision-makers with prompt techno-economic and policy insights on the reliability of these technologies under varied market scenarios.

5. Conclusions

In response to escalating uncertainties within final markets, the need for adaptive decision-making methodologies has become increasingly imperative. Agent-based modelling has proven to be a powerful approach, capable of efficiently exploring multiple cases and scenarios, thus facilitating expedited and well-informed decision-making processes within limited timeframes. This study employed ABM to examine the allocation of natural gas to various utilisation routes under diverse network configurations and economic and environmental scenarios. By simulating four main cases and two sub-scenarios for each case, distinct patterns of resource allocation were observed, and key factors influencing the decision-making process were identified. Primarily, the selection of utilisation routes within the network dictates the allocation strategy, which is subsequently refined by economic or environmental constraints while adhering to operational limitations. These factors collectively influence the system's resource allocation dynamics. Notably, cases prioritising fulfilling power requirements exhibited a lower average annual profitability than those focused on exporting natural gas monetisation. Specifically, case 4, which incorporated power generation, experienced a significant reduction in average annual profitability by approximately 47%, resulting in $2.77 billion, compared to $5.22 billion in case 3, which excluded power generation. Case 3 demonstrated the highest profitability across both economic and environmental scenarios but also registered the second-highest emissions (0.66 CO_2eq t/y), following case 2 under the economic scenario, which emphasised hydrogen-rich process routes.

The data-driven framework presented herein functions as a robust decision-making tool designed to respond to uncertainties effectively. By leveraging real-time data and employing adaptive algorithms, this framework empowers decision-makers to flexibly adjust strategies in response to fluctuating market conditions, thereby enhancing organisational agility and resilience. However, it is important to note that the results of this study do not account for contractual obligations where sellers are required to provide buyers with fixed capacities over the contract duration. Future research should consider integrating such contractual constraints to offer a more comprehensive understanding of resource allocation dynamics in real-world scenarios. Additionally, the economic scenario analysis is predominantly driven by global demand and forecasted selling prices of each commodity, guided by annual forecasted prices and demand, without incorporating segmented pricing systems utilised for specific commodities, such as LNG. Future studies should aim to integrate segmented pricing dynamics to provide a more nuanced understanding of resource allocation strategies.

CRediT authorship contribution statement

Noor Yusuf: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis. **Ahmed AlNouss:** Conceptualization, Methodology, Investigation, Formal analysis, Writing – review & editing. **Roberto Baldacci:** Conceptualization, Methodology, Investigation, Writing – review & editing, Supervision. **Tareq Al Ansari:** Conceptualization, Methodology, Writing – review & editing, Supervision, Resources, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors do not have permission to share data.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.ecmx.2024.100734.

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