Agent-Based Simulation Modeling for Sustainable Chemical Production and Resource Management

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Abstract: This study investigates the optimization of resource allocation and energy efficiency within a sustainable chemical production network using three distinct methods: Resource Availability-Based Selection, Pareto-based Selection, and Pareto Optimization. Each method was analyzed based on its ability to manage energy consumption, production efficiency, and resource utilization across multiple iterations. The Resource Availability-Based Selection method prioritized available resources in storage, while the Pareto-based Selection introduced input price considerations. Pareto Optimization, the most advanced approach, balanced production efficiency and cost-effectiveness, resulting in the highest overall performance. Findings demonstrate that multi-objective optimization, particularly Pareto Optimization, enhances operational efficiency and sustainability. The study's implications suggest adopting advanced optimization strategies to achieve energy efficiency and sustainability goals in the chemical industry. Additionally, recommendations for future research include incorporating real-time market dynamics, logistical factors, and renewable energy sources into the model to further enhance decision-making.

1 INTRODUCTION

In recent years, the chemical industry has faced increasing pressure to adopt more sustainable practices due to environmental and economic considerations. Sustainable chemical production (SCP) minimizes environmental impact while optimizing resource utilization, ensuring long-term viability (Haleem et al., 2023; Mishra et al., 2023). Traditional evaluation methods often fail to capture the complexity of interactions in production systems. To address this, the purpose of this study is to develop and analyze an agent-based modeling and simulation (ABMS) framework for sustainable chemical production and resource management. By simulating interactions between production facilities, markets, and resource providers, the study aims to optimize production processes, reduce waste, and enhance sustainability.

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2 LITERATURE REVIEW

Agent-Based Modeling and Simulation (ABMS) has emerged as a powerful tool for analyzing complex systems, particularly in resource allocation and supply chain management. Its ability to model autonomous agents and their interactions provides valuable insights into system dynamics and performance.

In supply chain networks, ABMS has been integrated with the Supply Chain Operations Reference (SCOR) model to enhance the modeling of distributed supply chain systems (Long, 2014). This integration allows for a more comprehensive analysis of supply chain processes and performance metrics. Additionally, ABMS has been combined with reinforcement learning to optimize stochastic supply chains, particularly in managing supplier disruptions (Aghaie and Hajian Heidary, 2019). This simulation-based optimization approach has proven effective in handling uncertainties within supply chains. Furthermore, ABMS has been applied to model Liquefied

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Natural Gas (LNG) import terminals, demonstrating its effectiveness in supply chain management for energy sectors (Venkataramanan and Srinivasan, 2024). These studies highlight the capability of ABMS to evaluate real-world scenarios and disruptions, reinforcing its value in complex supply chain management.

In chemical production, ABMS enables the exploration of various scenarios, including the effects of different resource management strategies on production efficiency and environmental sustainability (Helo and Rouzafzoon, 2023; Zhou et al., 2024). This capability is particularly valuable in the context of sustainable development, where ABMS facilitates the balancing of economic, environmental, and social objectives. Additionally, ABMS supports the integration of real-time data and adaptive strategies, making it a powerful tool for managing dynamic and complex industrial environments (Ionescu et al., 2024). Recent studies have demonstrated its effectiveness in optimizing production processes, enhancing resource allocation, and improving decision-making under uncertainty (Zhu et al., 2023).

These studies collectively demonstrate the versatility and efficacy of ABMS in addressing various challenges in resource allocation and supply chain management. By capturing the behaviors and interactions of individual agents, ABMS facilitates a deeper understanding of complex systems, leading to more informed and effective decision-making.

3 CASE STUDY: SCP MODEL

The sustainable chemical production (SCP) model is a comprehensive agent-based simulation framework designed to optimize and manage chemical production and resource allocation within an industrial ecosystem. The model is composed of various interconnected components and agents, each representing a specific function within the system. The primary agents in the SCP model include facilities (such as reactors, storage units, and treatment plants), markets, and suppliers. Each facility agent is characterized by its input and output materials, storage capacities, operational costs, and production scales (Figure 1). The model simulates the dynamic interactions between these agents, focusing on their decision-making processes related to purchasing raw materials, producing goods, and selling outputs in response to market conditions.

Figure 1 illustrates the structural components and interactions within the SCP model, emphasizing resource flows between key agents such as facilities

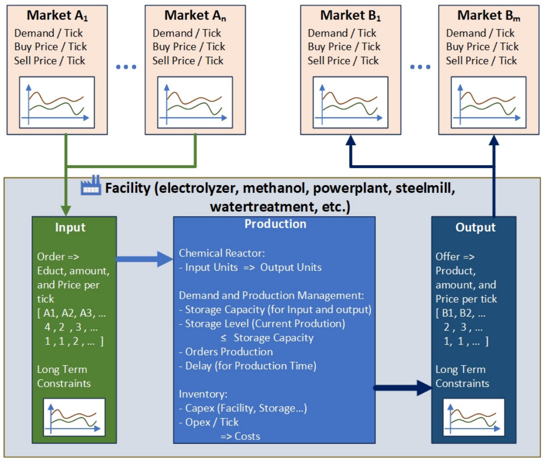

Figure 1: Resource Flow and Decision-Making in the SCP Model. The diagram illustrates the exchange of raw materials, intermediate products, and final outputs among facilities, markets, and suppliers, highlighting key interactions in production, purchasing, and sales.

(e.g., methanol plants, electrolyzers), markets, and suppliers. Arrows represent the movement of raw materials (e.g., CO_2, H_2, coal), intermediate products (e.g., methanol, treated water), and final outputs. The model integrates dynamic decision-making for purchasing, production, and sales while ensuring that storage levels remain within capacity limits. By capturing resource exchanges alongside market interactions, this representation underscores the model's capability to optimize resource allocation, production efficiency, and sustainability in chemical production.

Remarks on Markets:

- Prices derive from time series (selling prices typically differ from purchase prices). Each product's price (e.g., for CO_2) is dynamically derived from time series data sourced directly from external files, allowing for realistic variations over time.
- Demand is influenced by factors that are represented through time series data.

Remarks on Input Facility:

- Demand is decided from own production, use of storage, and market purchases.
- Demand is influenced by factors represented in a time series.
- Long-term constraints can necessitate purchases (e.g., purchase contracts).
- Market prices are influenced by factors that can be represented through time series data (which often differ from selling prices).

Remarks on Output Facility:

- Production is limited by facility capacity.
- Selling price is calculated as Totex (Capex + Opex), with Opex influenced by input prices.
- Long-term constraints may necessitate production despite unfavorable market prices (e.g., supply contracts).
- Market prices are influenced by factors that can be represented through time series data (which often differ from purchase prices).

In industrial financial modeling, the selling price of a product is often calculated based on Totex, which consists of Capex (Capital Expenditure) and Opex (Operational Expenditure). Capex represents the investment in long-term assets, such as infrastructure, while Opex covers the ongoing costs of production, including input prices. Opex is particularly sensitive to fluctuations in market prices for raw materials and energy, making it a dynamic component. By combining Capex and Opex, Totex reflects the total cost of ownership, guiding pricing strategies to ensure profitability and sustainability. This comprehensive approach aids in financial planning and resource management.

Facilities within the SCP model, such as methanol plants and electrolyzers, play crucial roles in transforming raw inputs into valuable chemical products. For example, the methanol facility converts carbon dioxide (CO_2) and hydrogen (H_2) into methanol (CH_3OH) and water (H_2O), while the electrolyzer facility produces hydrogen from water using electricity (Figure 2). These facilities operate under constraints such as production times, capacities, and economic factors like operating expenses and market prices. The model uses advanced decision-making algorithms, including Pareto-based selection and Pareto Optimization, to optimize the facilities' operations, ensuring efficient resource use and maximizing economic returns. This holistic approach allows the SCP model to provide insights into the sustainability and economic viability of chemical production processes, making it a valuable tool for industrial resource management.

Figure 2 provides a detailed view of various facilities within the SCP model, including methanol facilities, electrolyzer, power plant, steel mill, and water treatment. It showcases the input and output relationships for these facilities, such as the coal market input and power and CO_2 market outputs for the power plant. This illustration highlights how the model is generalized to other facilities like ethanol, urea, and biomass, offering a comprehensive depiction of the interconnected industrial ecosystem.

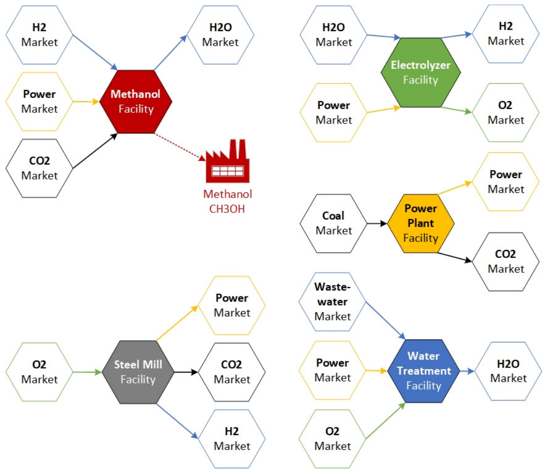

Figure 2: Real-world Representation of Facility Interactions.

The SCP model is chosen for its comprehensive approach to simulating and optimizing chemical production and resource management. Its ability to incorporate various facilities such as methanol plants, electrolyzers, power plants, and water treatment units allows for a detailed analysis of the interactions between different production processes and resource flows. By simulating these interactions, the SCP model helps identify inefficiencies and opportunities for optimization, making it a powerful tool for enhancing sustainability in chemical production.

In the broader context of sustainable chemical production, the SCP model addresses critical challenges such as resource utilization, energy efficiency, and environmental impact. By integrating real-time data and adaptive decision-making strategies, the model provides insights into how different production strategies affect overall sustainability. This holistic perspective is essential for developing practices that balance economic, environmental, and social objectives, aligning with the goals of sustainable development. The SCP model's ability to simulate complex industrial ecosystems and optimize resource management makes it a valuable asset in the pursuit of sustainable chemical production.

4 METHODOLOGY

4.1 Agent-Based Simulation Modeling

Agent-Based Modeling and Simulation (ABMS) is a computational framework that enables the representation of autonomous agents, each with distinct attributes and decision-making capabilities, to simulate interactions within a system. In the context of sustainable chemical production, ABMS provides a detailed and dynamic representation of industrial facilities, markets, and resource flows. This approach is particularly valuable for capturing the complexity of interconnected industrial ecosystems, where multiple facilities, such as methanol plants, electrolyzers, and power plants (Figure 3), interact through material and energy exchanges. By simulating these interactions, ABMS allows for an in-depth analysis of production processes, resource allocation, and market dynamics. This capability is essential for evaluating the impact of different decision-making strategies on resource utilization, energy efficiency, and overall environmental sustainability, making ABMS a powerful tool for optimizing industrial operations in real-world scenarios.

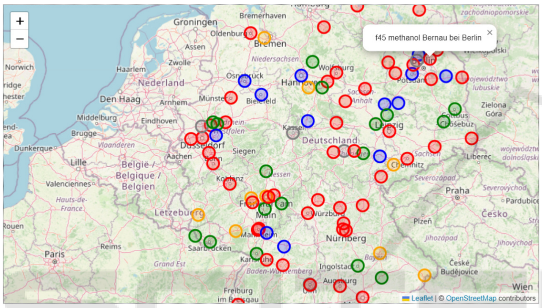

Figure 3: Geospatial Distribution of Facilities.

Figure 3 presents the geospatial distribution of facilities introduced in Section 3, illustrating their spatial relationships within the industrial ecosystem. Each facility is represented by a colored circle, maintaining consistency with the color scheme in Figure 2, to depict its location. This spatial representation enables the analysis of logistical constraints, transportation costs, and regional resource availability, which influence decision-making within the simulation. The geospatial component is implemented using MESA-GEO's `GeoSpace()` function in Python, allowing facilities to interact dynamically based on their locations. By incorporating spatial constraints, the model ensures a more realistic representation of industrial operations, considering factors such as material transportation and facility proximity in resource allocation strategies.

During each simulation run, market and facility agents are activated in a partially randomized order, consistent with standard agent-based modeling approaches. Market agents, such as the hydrogen market, operate passively without initiating actions or making independent decisions. Instead, they serve as intermediaries that regulate economic interactions within the simulation. Their primary functions include calculating new prices at each time step based on historical time series data, generating statistical insights at the market level rather than for individual facilities, and managing market offers, effectively acting as a centralized commodity exchange. By maintaining an updated list of market offers, these agents provide a structured platform for facilities to engage in transactions, ensuring a realistic representation of industrial market dynamics.

Facility agents, such as electrolyzers, actively engage in decision-making and execute key operational processes. These agents determine their output product offers, setting quantities and prices before listing them on the market, while also incorporating spatial attributes such as location to account for transportation costs and delivery times. Additionally, facility agents procure necessary input materials by selecting from market offers based on predefined needs, preferences, and optimization strategies, including Pareto-based selection. Their role extends beyond market interactions, as they continuously initiate production cycles, converting inputs into outputs at rates defined by industrial profiles contributed by project partners. This dynamic decision-making structure allows the simulation to capture the complexities of industrial operations, resource management, and economic behavior within a multi-agent system.

The objective of the simulation is to analyze system-wide developments when each facility agent independently optimizes its own outcomes while being influenced by market conditions. Facility agents operate autonomously, making decisions based on production efficiency, cost minimization, and resource availability. Their interactions are shaped by market forces, particularly through pricing and supply fluctuations, reflecting real-world industrial dynamics. Additionally, facilities can establish long-term agreements, fostering strategic partnerships that influence resource allocation and production efficiency. These interactions may lead to the emergence of production clusters or supply chains that naturally develop under given conditions. By identifying such emergent patterns, the simulation provides valuable insights into industrial self-organization, supporting the design of more efficient and resilient production networks.

In the ABMS framework, reactors simulate the transformation of raw materials and energy into products across industrial facilities. Their efficiency depends on production capacity, technological constraints, and market conditions like resource availability and pricing. This dynamic interaction enables realistic modeling of industrial operations and resource optimization. Table 1 outlines reactor configurations, detailing inputs and outputs that drive the simulation.

Market agents play a crucial role in managing price dynamics, regulating the availability of goods, and facilitating transactions within the simulation. The system distinguishes between input and output prices, incorporating market fluctuations into the decision-making processes of facility agents. This integration ensures that pricing strategies reflect real-world economic conditions, allowing agents to respond dynamically to changing supply and demand. By enabling strategic interactions and accounting for price volatility, the market framework enhances the adaptability and realism of the model, providing a more accurate representation of industrial market behavior.

ABMS enables the integration of real-time data and adaptive decision-making, which are essential for optimizing chemical production processes. By simulating various scenarios and their long-term effects, ABMS helps identify strategies that balance economic viability with environmental and social objectives. Its ability to model complex systems, capture dynamic interactions, and provide comprehensive analyses makes it a valuable tool for advancing sustainable chemical production. This approach supports the development of optimized production strategies that enhance resource efficiency while minimizing environmental impact, offering insights beyond those achievable through traditional modeling methods.

4.2 Model Specifications

The Sustainable Chemical Production (SCP) model is designed with specific agents, behaviors, interactions, and environmental contexts to simulate and optimize chemical production processes.

Agent Behavior. Each facility within the model acts as an autonomous agent with unique properties and decision-making processes. For example, a methanol plant agent has attributes (Figure 2) such as input materials (e.g., CO_2 and H_2), output products (e.g., methanol and water), production capacity, and operational costs as stated in Section 3. These agents follow specific rules and algorithms to decide on the purchase of raw materials, the quantity of production, and the sale of finished goods.

Interactions. Interactions between agents are governed by market dynamics and resource flows. Facilities interact with market agents to procure raw materials and sell their products. For instance, the power plant facility buys coal from the market and sells power and CO_2 (Figures 1 and 2). These transactions are influenced by market prices, availability of resources, and contractual obligations. The model also simulates internal interactions where outputs from one facility (e.g., hydrogen from the electrolyzer) serve as inputs for another (e.g., methanol production).

Environment. The model operates within a simulated industrial ecosystem that includes various markets and environmental factors. Markets are modeled to provide time-series data on prices and demand, ensuring realistic economic conditions. Environmental constraints such as storage capacities, production limits, and resource availability are defined in the facilities' configuration files and actively enforced during simulations to reflect real-world limitations. This ensures agents operate within these constraints, dynamically adjusting their decisions based on factors like available storage space and production capabilities. Additionally, the model's environment accounts for long-term constraints such as purchase and supply contracts, which influence facility operations and decision-making processes (Figure 3).

By incorporating detailed agent behaviors, complex interactions, and realistic environmental conditions, the SCP model provides a comprehensive framework for analyzing and optimizing sustainable chemical production processes. This enables the identification of strategies that enhance resource efficiency, reduce environmental impact, and ensure economic viability.

4.3 Data Collection

The data collection process in this agent-based modeling and simulation (ABMS) involves gathering and analyzing key variables to understand the dynamics of sustainable chemical production. The model utilizes the MESA framework in Python, which allows for the simulation of complex interactions between various agents, including facilities and markets. Data collection is integrated within the simulation process, capturing detailed information at each step of the model's execution.

4.3.1 Sources and Methods of Data Collection

Data are collected from several sources, including the internal states of agents (such as production levels, energy consumption, and storage capacities) and external market factors (like price fluctuations and demand). The simulation continuously gathers data on these variables throughout the iterations, enabling a comprehensive analysis of the system's behavior over time. Key metrics such as total energy consumed, total energy produced, and financial transactions (purchases and sales) are tracked using MESA's built-in

Table 1: Summary of Reactor Inputs and Outputs in Various Facilities.

Facility	Input	Output	Reactor Type
Methanol Plant (Sollai et al., 2023)	CO_2, H_2, Power	CH_3OH, H_2O	Chemical
Electrolyzer (El-Shafie, 2023)	H_2O, Power	H_2, O_2	Electrolysis
Power Plant (Okunlola et al., 2023)	Coal	CO_2, Power	Combustion
Steel Mill (Singh et al., 2022)	O_2	H_2, CO_2, Power	Metallurgical
Water Treatment (Fadillah et al., 2024)	Wastewater, Power, O_2	H_2O	Filtration

`DataCollector()` functionality. This data is then stored for further analysis and visualization, allowing for the assessment of performance indicators critical to sustainable chemical production. The collected data provides insights into the efficiency of different strategies and helps identify areas for optimization within the system.

4.4 Algorithm

Following the detailed specifications of the agents in Section 4.2, the core computational framework for the simulation is described using an algorithm that governs how facilities and markets interact, allocate resources, and optimize production. The algorithm serves as the backbone for managing agent behavior, resource flows, and decision-making within the simulation environment.

The simulation model operates by first initializing all agents, facilities such as methanol plants, power plants, and water treatment plants, as well as markets for key commodities like carbon dioxide (CO_2), water (H_2O), hydrogen (H_2), oxygen (O_2), wastewater, and coal. The agents operate based on their defined roles, interacting through the market system to purchase or sell resources. The algorithm for resource optimization in the simulation is broken down into the following steps:

1. **Initialize Agents and Markets.** At the beginning of each simulation run, facilities and markets are initialized based on predefined configurations stored in external JSON files. Each facility in the SCP model (Sections 3 and 4) is assigned operational parameters, including input requirements, production capacity, available storage, and financial characteristics. Markets are dynamically influenced by time series data sourced from external CSV files and account for fluctuating material prices, providing realistic price variability for agents' decision-making.
2. **Resource Availability Check.** Facilities assess their available resources stored onsite, such as water, CO_2, wastewater, and coal, and determine their current production capabilities based on resource availability. This step ensures that the production level does not exceed what is sustained by the available inputs.
3. **Market Interaction.** Each facility engages with the market to purchase the required resources if the current storage is insufficient. Facilities also sell their output (e.g., methanol, power) to the respective markets. Prices and availability in the market influence these transactions, following a Pareto optimization or resource-based selection method.
4. **Production and Optimization.** Once the necessary resources are secured, the facility initiates production, with output levels adjusted according to the "Resource Availability-Based Selection", "Pareto-based Selection", or "Pareto Optimization" strategies (outlined in Sections 5.1.1 to 5.1.3). For instance:
   - In the *Resource Availability-Based Selection*, production is directly tied to the amount of resources available in storage.
   - In the *Pareto-based Selection* and *Pareto Optimization* methods, production decisions are based on balancing multiple factors like input costs and resource availability to maximize efficiency.
5. **Data Collection and Analysis.** After each simulation step, the system collects data (Section 4.3) on key variables such as total energy consumed, total energy produced, prices of purchased and sold resources, and the amount of materials traded in the market. These values are recorded for later analysis to measure the performance of each method over the simulation iterations.
6. **Repeat Process.** The simulation iterates through multiple steps, where agents continuously assess their resource needs, engage in the market, and adjust production outputs, reflecting real-world industrial processes.

The algorithm implements a multi-objective optimization strategy, with a particular focus on the Pareto-based methods that balance trade-offs between cost minimization and production maximization. This approach to structured decision-making enables the simulation to identify optimal strategies for resource allocation, supporting sustainable chemical production objectives. By detailing this computational framework, the algorithm systematically models agent interactions and operations within the SCP model, accurately simulating real-world industrial processes while effectively integrating resource constraints and market dynamics.

5 RESULTS AND DISCUSSION

This section presents the findings from simulating three decision-making methods in a cross-industrial network for sustainable chemical production. The simulation, conducted over 100 iterations per method, evaluates key metrics such as energy consumption, production efficiency, price sales, and purchases across various facilities, including methanol plants, electrolyzers, power plants, steel mills, and water treatment units. Data outputs were systematically recorded in CSV files, capturing facility-market interactions. The model incorporates a diverse range of industrial facilities, differentiated by scale and capacity, to reflect real-world operations. It includes 40 methanol production plants (25 small, 10 medium, and 5 large), 20 electrolyzers (15 small, 5 medium), 12 medium-sized power plants, 5 large steel mills, and 10 medium water treatment facilities. These configurations, informed by industrial data, contribute to a realistic representation of an interconnected industrial ecosystem. Figure 3 visualizes the spatial distribution of these facilities within the simulation environment.

5.1 Simulation Outputs

5.1.1 Resource Availability-Based Selection

The Resource Availability-Based Selection method optimizes facility operations by adjusting production output to match the availability of resources in storage. By ensuring that the facility's inputs are aligned with current storage levels, this method reduces the risk of resource overuse or shortages, promoting efficient and stable production. It focuses on balancing input availability with production demands, making it well-suited for environments where maintaining continuous operation without disruptions is a priority. This approach operates independently of external market factors, such as fluctuations in input prices.

In the method, the production output of a facility is determined by aligning available resource levels with the required reactor inputs for production. The production process is generalized as follows:

$$P_{output} = \min\left(\frac{R_{input1}}{r_{input1}}, \frac{R_{input2}}{r_{input2}}, \ldots\right)$$

Where:

- P_{output} represents the maximum production output, such as methanol, power, or other products depending on the facility.
- $R_{input1}, R_{input2}, \ldots$ denote the available quantities of required resources (e.g., carbon dioxide, hydrogen, water, or coal) in the facility's storage.
- $r_{input1}, r_{input2}, \ldots$ represent the input requirements for each resource per unit of production.

For example, a methanol facility requires reactor inputs like carbon dioxide, hydrogen, and power, while a power plant primarily relies on coal. This method identifies the bottleneck resource for any facility and adjusts the production output accordingly, ensuring efficient use of available resources without exceeding operational constraints.

During the steps, this method demonstrated a steady increase in both energy consumption and production, though its overall efficiency plateaued when compared to more advanced optimization techniques. Energy consumption grew from 5,299 megawatt-hours (MWh) at the start to over 508,000 MWh by the final iteration, while energy production reached 254,485 MWh (Table 2). Additionally, the total amount of carbon dioxide purchased consistently exceeded the amount sold, with the gap widening as the number of iterations increased (Figure 4).

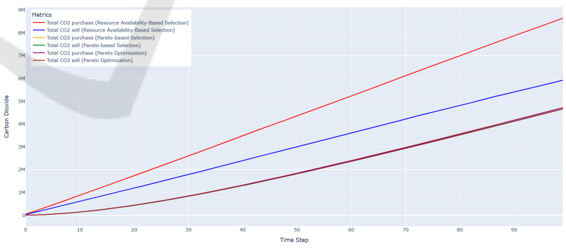

Figure 4: Comparison of Total CO_2 Purchase and Sell in Three Methods.

In conclusion to this section, clarifying the abbreviations and measurement units in Tables 2, 3, and 4 is essential to maintain consistency and facilitate clear interpretation of the data presented. "Total Energy Consumed" refers to the energy used by the facilities, measured in megawatt-hours (MWh), while "Total Energy Produced" indicates the energy generated by the facilities, also measured in MWh. The tables also report water transactions, with "Total H_2O Purchase" and "Total H_2O Sell" reflecting the quantities of water purchased and sold, measured in liters (L).

Table 2: Summary Statistics of Energy, Prices, and Material Transactions (Resource Availability-Based Selection method).

Field	Min	Max	Mean	Std Dev
Total Energy Consumed (MWh)	5,299.0	508,280.6	265,912.4	144,395.2
Total Energy Produced (MWh)	2,231.8	254,485.6	127,184.9	73,861.7
Total H_2O Purchase (L)	22,473.0	2,183,441.9	1,172,773.8	614,694.2
Total H_2O Sell (L)	13,369.2	2,160,537.2	1,088,608.8	625,706.8
Total H_2 Purchase (m^3)	2,696.9	1,388,470.3	687,796.8	412,387.1
Total H_2 Sell (m^3)	7,737.3	2,161,159.4	1,074,404.4	641,651.2
Total O_2 Purchase (m^3)	8,452.8	3,977,244.7	1,891,612.6	1,185,319.0
Total O_2 Sell (m^3)	13,242.7	4,064,658.7	1,980,978.3	1,193,471.9
Total CO_2 Purchase (m^3)	49,811.8	8,642,920.5	4,323,469.0	2,521,670.9
Total CO_2 Sell (m^3)	34,190.0	5,923,805.7	2,977,017.8	1,731,421.6
Total CH_3OH Sell (m^3)	7,838.0	4,204,812.0	2,029,045.8	1,235,886.6
Total Coal Purchase (kg)	5,655.8	802,230.4	403,925.5	231,973.2
Total Wastewater Purchase (L)	10,494.0	1,883,808.0	956,280.2	543,677.6
Total Price Sales (Euro)	632,019.8	207,936,053.7	103,164,904.6	60,782,915.7
Total Price Purchases (Euro)	2,608,095.5	376,430,049.9	189,182,797.3	109,385,501.7

For gases like hydrogen, oxygen, and carbon dioxide, the terms "Total H_2 Purchase/Sell", "Total O_2 Purchase/Sell", and "Total CO_2 Purchase/Sell" denote the quantities of these gases traded in cubic meters (m^3). Similarly, "Total CH_3OH Sell" represents methanol sold in cubic meters (m^3), "Total Wastewater Purchase" specifies the volume of wastewater acquired, measured in liters (L), while "Total Coal Purchase" specifies the amount of coal acquired, measured in kilograms (kg). "Total Price Sales" represents the total revenue generated from sales in euros, and "Total Price Purchases" captures the total expenditure on purchasing resources, also in euros. These clarifications ensure the correct interpretation of the numerical data in the corresponding tables. To ensure clarity in interpreting the table data, the first line of each table includes the columns "Field", "Min" (minimum values), "Max" (maximum values), "Mean" (average values), and "Std Dev" (standard deviation). This structure provides a comprehensive view of the data's range and variability, supporting detailed analysis of each field's statistical distribution.

5.1.2 Pareto-Based Selection

In the Pareto-based Selection method, production optimization is achieved by considering both resource availability and market prices. Mathematically, the production amount P is determined by the available amounts of each resource R_i, their respective input requirements I_i, and the market price M_i for each resource. The potential production limits L_i for each resource i are calculated as:

$$L_i = \frac{R_i}{I_i},$$

Next, the bottleneck resource is identified as the one with the smallest production limit, which sets the maximum feasible production amount:

$$P_{max} = \min(L_i),$$

This maximum production amount is further adjusted by considering the influence of market prices. The final production amount $P_{adjusted}$ is calculated by taking the minimum of the production amount and the price-adjusted resource availability:

$$P_{adjusted} = \min(\frac{R_i}{I_i.M_i}),$$

Here, R_i represents the available resource quantity, I_i the input requirement for each unit of production, and M_i the market price for the resource. This optimization ensures that production is both cost-efficient and resource-efficient, balancing the availability of resources and economic factors.

This approach led to a marked increase in total energy consumption and production, with energy output in later stages reaching up to $6,640$ MWh. Additionally, total sales and purchases were significantly higher, reflecting heightened economic activity within the system. By integrating both market dynamics and resource constraints, this strategy enabled more effective resource utilization. Notably, the simulation showed that energy production was approximately one-quarter of energy consumption, with the total energy consumed reaching $21,329$ MWh and energy produced at $6,640$ MWh by the final iteration (Table 3). Furthermore, the quantities bought and sold for key commodities, such as carbon dioxide, water, hydrogen, and oxygen, remained nearly balanced (Figure 5), indicating stable trading patterns across multiple iterations. For instance, the total amounts of carbon dioxide purchased and sold were closely aligned, a trend also observe for other commodities, with minimal variation over repeated cycles.

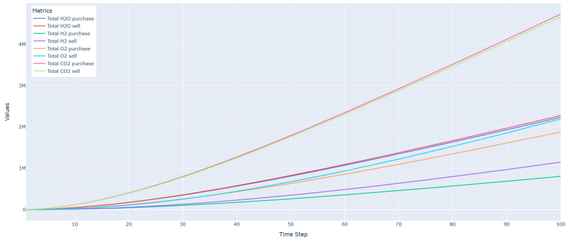

Figure 5: Commodity Transactions (Water, Hydrogen, Oxygen, and CO_2) Across Iterations for Pareto-based Selection.

5.1.3 Pareto Optimization

The Pareto Optimization method employs multi-objective optimization to balance resource procurement, production, and sales while ensuring Pareto efficiency where no resource is improved at the expense of another. This approach minimizes procurement costs, maximizes production efficiency, and optimizes profits while accounting for constraints such as storage capacity, market prices, demand fluctuations, and resource availability. The production amount P is determined by balancing available resources R_i, input requirements I_i and market prices M_i. Initially, the available resources are adjusted for market price differences, yielding the price-weighted resource availability:

$$R_i' = \frac{R_i}{M_i},$$

Next, the ratios ρ_i of available resources to their input requirements are calculated as:

$$\rho_i = \frac{R_i'}{I_i},$$

The bottleneck resource, which has the smallest ratio, limits the production amount. Thus, the maximum production amount P_{max} is given by the resource with the smallest ratio:

$$P_{max} = \min(\rho_i),$$

This method ensures a Pareto-efficient production, meaning no single objective (e.g., minimizing cost or maximizing output) is improved without worsening another. By factoring in both resource availability and price adjustments, the method achieves optimal resource utilization and economic performance.

The algorithm first calculates resource availability relative to market prices, giving priority to more affordable resources. It then determines the maximum feasible production amount by identifying bottleneck resources, which are the limiting factors in production. The Pareto optimization balances resource allocation based on these constraints, ensuring that the selected production plan optimizes cost-effectiveness and production efficiency. This approach is more sophisticated than basic selection methods as it integrates market dynamics and capacity limits, ultimately leading to an efficient allocation of resources across the facility network.

This approach achieved the highest total price sales and the lowest price purchases, optimizing the balance between energy consumption and production. For example, in the final stages of the simulation, total energy consumption surpassed $10,842$ MWh, while total energy production reached $5,565$ MWh (Table 4). Notably, this optimization technique led to a considerable reduction in raw material purchases, which positively impacted the operational cost and resource utilization across the network. Similar to the Pareto-based Selection method, the purchase and sell in this approach follow a balanced and systematic resource allocation process (Figure 6). However, in terms of energy consumption and production, the Pareto Optimization method demonstrates a superior efficiency, achieving more optimal energy usage than other methods (Figure 7).

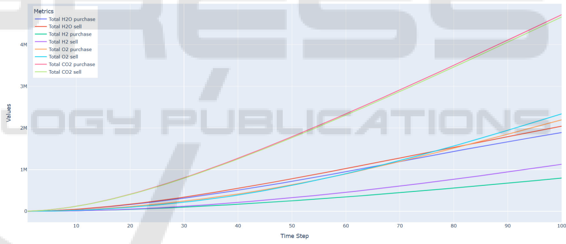

Figure 6: Commodity Transactions (Water, Hydrogen, Oxygen, and CO_2) Across Iterations for Pareto Optimization.

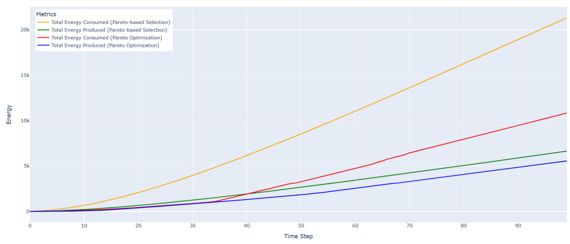

Figure 7: Comparison of Energy Purchase and Sell in Pareto-based Selection and Pareto Optimization Methods.

Each method displayed distinct trade-offs between energy efficiency, production capacity, and economic performance, making the Pareto Optimization approach the most effective strategy for sustainable production. The results indicate that advanced decision-making methods can significantly re-

Table 3: Summary Statistics of Energy, Prices, and Material Transactions (Pareto-based Selection).

Field	Min	Max	Mean	Std Dev
Total Energy Consumed (MWh)	11.0	21,329.4	9,078.5	6,612.2
Total Energy Produced (MWh)	4.0	6,640.6	2,829.5	2,055.5
Total H_2O Purchase (L)	984.9	2,232,767.8	915,167.9	690,953.1
Total H_2O Sell (L)	1,012.1	2,277,045.6	933,788.2	704,521.6
Total H_2 Purchase (m^3)	132.2	807,743.9	312,888.3	250,393.8
Total H_2 Sell (m^3)	268.7	1,149,619.6	430,642.3	356,096.9
Total O_2 Purchase (m^3)	397.0	1,879,904.0	740,961.1	582,796.3
Total O_2 Sell (m^3)	516.3	2,193,816.2	824,005.5	680,273.7
Total CO_2 Purchase (m^3)	2,455.5	4,725,099.6	1,983,431.5	1,463,308.7
Total CO_2 Sell (m^3)	2,407.7	4,663,713.8	1,955,090.6	1,444,190.4
Total CH_3OH Sell (m^3)	40.9	2,095,473.4	699,146.8	648,522.5
Total Coal Purchase (kg)	267.0	475,919.5	202,648.7	147,454.9
Total Wastewater Purchase (L)	673.2	1,197,079.5	509,335.3	370,882.9
Total Price Sales (Euro)	16,518.9	138,659,035.2	48,956,108.98	42,909,722.9
Total Price Purchases (Euro)	122,871.4	223,658,461.6	95,048,939.4	69,299,005.8

Table 4: Summary Statistics of Energy, Prices, and Material Transactions (Pareto Optimization).

Field	Min	Max	Mean	Std Dev
Total Energy Consumed (MWh)	0.0	10,842.7	4,001.4	3,511.0
Total Energy Produced (MWh)	0.0	5,565.6	2,171.4	1,736.1
Total H_2O Purchase (L)	846.0	1,888,945.6	801,317.3	594,864.5
Total H_2O Sell (L)	882.0	2,042,219.5	861,946.5	639,048.3
Total H_2 Purchase (m^3)	130.3	797,192.7	302,807.7	245,726.9
Total H_2 Sell (m^3)	260.6	1,128,242.0	409,677.3	347,200.5
Total O_2 Purchase (m^3)	343.0	2,194,182.1	807,061.6	678,033.65
Total O_2 Sell (m^3)	446.0	2,337,957.8	823,313.3	721,073.3
Total CO_2 Purchase (m^3)	2,418.9	4,716,858.8	1,979,621.4	1,459,026.9
Total CO_2 Sell (m^3)	2,418.9	4,661,324.5	1,954,031.7	1,441,608.1
Total CH_3OH Sell (m^3)	0.0	2,078,860.0	688,369.8	644,578.1
Total Coal Purchase (kg)	252.7	474,804.7	202,517.3	147,283.7
Total Wastewater Purchase (L)	540.0	1,092,150.0	474,468.3	342,149.0
Total Price Sales (Euro)	12,347.7	131,024,730.2	45,056,517.7	40,638,311.4
Total Price Purchases (Euro)	114,409.6	221,473,197.2	94,073,347.6	68,913,709.8

duce costs and improve resource utilization in the industrial networks.

5.2 Analysis

The Resource Availability-Based Selection method shows a steady rise in energy consumption and production over the iterations (Section 5.1.1). However, its efficiency plateaus when compared to more advanced methods. This behavior is attributed to the method's dependence on available resources in storage, which, although ensuring that the facility does not exceed its input constraints, limits optimization potential. The method lacks flexibility in handling dynamic market prices or external factors, making it less responsive to changes in resource costs. As a result, energy consumption increases to 508,000 MWh by the final step, while energy production peaks at 254,485 MWh. Additionally, discrepancies in material transactions, particularly in CO_2 purchases and sales, highlight the limitations of this approach in balancing resource inflows and outflows effectively.

The Pareto-based Selection method, designed to optimize production by considering both resource availability and market prices, demonstrates significant improvements in efficiency (Section 5.1.2). This approach achieves better resource allocation by minimizing costs and maximizing production outputs. For instance, by factoring in market dynamics, the method maintains a closer balance between energy consumption and production, with the final energy consumption exceeding 21,000 MWh and production reaching

6,640 MWh. Material transactions, such as water, hydrogen, oxygen, and carbon dioxide, show more stability in terms of purchase and sell quantities, leading to more balanced operations. The results confirm that the Pareto-based approach outperforms simpler resource allocation strategies by effectively leveraging market conditions alongside resource availability.

The Pareto Optimization method further refines the multi-objective approach by focusing on maximizing production efficiency while minimizing operational costs (Section 5.1.3). This method consistently produces the most optimal results, with energy consumption reaching over 10,800 MWh and energy production nearing 5,565 MWh by the final step. Notably, the method achieves a significant reduction in raw material purchases compared to the previous approaches, as it strategically prioritizes cheaper resources and ensures that each production decision is Pareto-optimal. This leads to overall improvements in network efficiency, with the total purchase and sell amounts for various commodities closely aligned. The superior performance of Pareto Optimization, in comparison to the other two methods, demonstrates its capability in managing resource constraints and market fluctuations effectively.

In conclusion, while all three methods have their merits, Pareto-based Selection and Pareto Optimization clearly outperform the Resource Availability-Based approach, particularly in scenarios involving dynamic markets. Pareto Optimization, in particular, achieves the most efficient balance between energy consumption, production, and material transactions, making it the most effective method for large-scale industrial applications.

5.3 Implications

The simulation framework developed in this study has significant implications for both sustainable chemical production and broader industrial applications. By employing the Resource Availability-Based Selection method, facilities can align production with available input resources, minimizing energy consumption and resource waste while improving overall efficiency. This approach reduces environmental impact, particularly in resource-intensive industries, by ensuring operations remain within input constraints. Similarly, the Pareto-based Optimization strategy enables facilities to balance multiple objectives, such as minimizing raw material purchases and maximizing production, ultimately lowering operational costs and emissions. These strategies enhance economic viability while promoting sustainability and regulatory compliance. Beyond chemical production, the framework's adaptability extends to industries such as logistics, energy, and supply chain management. In logistics, resource-aligned decision-making can optimize transportation routes and inventory control, reducing costs and inefficiencies. In the energy sector, Pareto-based optimization can balance energy generation and consumption based on resource availability, fuel costs, and environmental factors, providing a valuable tool for managing renewable energy fluctuations. Additionally, in global supply chains, where resource costs and availability vary regionally, the framework optimizes inventory levels and production schedules, ensuring efficient and sustainable operations. These diverse applications highlight the model's flexibility in improving resource management and sustainability across multiple industries.

5.4 Future Research

While this study provides valuable insights into resource optimization and energy efficiency in sustainable chemical production, several limitations highlight areas for future research. The model simplifies market conditions, assuming stable input prices and supply chains, which may not reflect real-world volatility. Additionally, it focuses on a limited set of materials, excluding catalysts, secondary emissions, and waste management complexities. Spatial assumptions, though accounting for geographic distribution, overlook transportation logistics and regional price variations critical for large-scale operations. Furthermore, the model does not distinguish between renewable and non-renewable energy sources or consider energy transmission losses, limiting its sustainability assessment. Economic and regulatory factors, such as taxes and subsidies, are also omitted, restricting its policy applicability. Future research should integrate dynamic market conditions, refine spatial logistics, incorporate renewable energy considerations, and expand material scope to enhance the model's realism and applicability in industrial sustainability.

6 CONCLUSIONS

This study explored the optimization of resource allocation and energy efficiency within sustainable chemical production networks using three distinct methods: Resource Availability-Based Selection, Pareto-based Selection, and Pareto Optimization. Each method demonstrated unique strengths in managing resource inputs and energy consumption. The Resource Availability-Based Selection method focused on aligning production output with available resources in storage, resulting in a steady increase in energy consumption and production over time. However, it exhibited limitations in maximizing efficiency compared to more advanced methods. The Pareto-based Selection method balanced input prices with resource availability, leading to more efficient production outcomes and higher economic activity. Lastly, the Pareto Optimization approach, as the most advanced method, consistently minimized operational costs while maximizing production efficiency, yielding the highest total price sales and demonstrating optimal energy use.

The findings highlight the significance of multi-objective optimization in improving resource management and production processes in chemical industries. By leveraging Pareto Optimization, companies can achieve a more balanced approach to energy use and resource allocation, ultimately enhancing both economic and environmental sustainability. However, the study also acknowledges that real-world complexities, such as market fluctuations and logistical constraints indicating areas for further improvement.

Based on the results, it is recommended that chemical production facilities adopt multi-objective optimization techniques like Pareto Optimization to enhance operational efficiency and sustainability. Future research should focus on incorporating dynamic market conditions, transportation logistics, and renewable energy sources into optimization models. Additionally, considering regulatory and economic factors, such as carbon pricing and subsidies, will offer a more comprehensive view of sustainability in chemical production. By adopting these improvements, industries can better align with global sustainability goals while maintaining economic viability.

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