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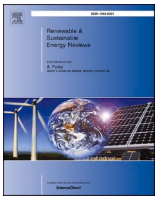

Techno-economic analysis and network design for CO₂ conversion to jet fuels in the United States

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ABSTRACT

The conversion of carbon dioxide (CO_2) into jet fuel holds significant potential for reducing CO_2 emissions, providing an alternative to carbon-based resources, and offering a renewable means of energy storage. The objective of this study is to conduct a techno-economic analysis and optimize the supply chain network for converting CO_2 to jet fuel in the United States, aiming to minimize total costs while assessing the environmental and economic feasibility of two CO_2 conversion pathways. This first pathway is based on Fischer-Tropsch synthesis (FTS), and the other one is based on the valorization and upgrading of light methanol (MeOH). Incorporating spatial and techno-economic data, a mixed-integer linear programming model was developed to select source plants and conversion pathways, locations of conversion refinery sites, and the amount of captured CO_2 across the United States. The optimal results indicate that the FTS pathway is adopted at all selected refineries when the hydrogen price is $1000/t and the operating cost, mainly electricity used in conversion, is reduced to 5 % of its current level. Under this scenario, the total annual profit is $8B and the net carbon emissions are −88,783,284 tons. The sensitivity analyses reveal that the prices of electricity and hydrogen significantly contribute to total production costs. The CO_2 recycle percentage of the FTS pathway influences the choice of applied pathways at refineries. Additionally, a higher conversion rate holds a substantial promise for reducing the total production cost and can make the MeOH pathway a viable choice.

1. Introduction

Converting carbon dioxide (CO_2) into fuels and chemicals not only promotes CO_2 reduction in the atmosphere but also provides alternative carbon-based resources and enables the storage of renewable energy [1]. However, large-scale CO_2 conversion faces significant technical and economic challenges in industrial applications. The net cost of CO_2 capture and utilization in some conventional conversion pathways might even surpass the value of the final products [2,3]. Capturing and storing CO_2 before conversion involves chemical transformations that require a substantial amount of energy input, significantly increasing the cost of CO_2 utilization. For example, reducing 810 Gt CO_2 from the atmosphere by 2100 under the current emissions scenario requires 111, 320 kWh of energy input, potentially exceeding the energy gained from burning fossil fuels emitting an equivalent quantity of CO_2 [4]. Research in catalyst selection, unit operation design, process configuration, life cycle assessment, environmental benchmarking, and policy analysis — all crucial aspects of CO_2 utilization — is still in its early stages [5,6].

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1.1. CO_2 conversion pathways

Current research efforts in CO_2 reduction have primarily concentrated on producing chemical products such as formic acid/formate, CH_4, methanol, ethylene, and ethanol, rather than focusing on fuels [7]. Direct drop-in liquid hydrocarbon fuels, including gasoline, diesel, jet fuels, and marine fuels, are promising candidates for meeting the growing demand for CO_2 reduction due to their large demand and high energy density. Recent advancements in CO_2 conversion technologies have seen significant progress in various areas, including catalysts, system integration, and innovative processes. Various approaches, such as photosynthetic, non-photosynthetic biological, electrochemical, photo-catalytic, thermochemical, and hybrid methods, can be employed to convert CO_2 to drop-in hydrocarbons [8–10]. Single-Atom Catalysts (SACs) have been highlighted for their high efficiency in converting CO_2 into valuable chemicals and fuels. These catalysts maximize atom utilization and provide unique electronic structures, improving catalytic performance and stability [11]. However, the long-term stability, scalability for industrial applications, mechanistic understanding of active sites, integration with renewable energy sources, and comprehensive environmental and economic assessments of SACs remain significant barriers. Advances in CO_2 reduction under hydrothermal conditions using renewable reductants have shown promise. This method aims for high efficiency and net carbon benefits by converting CO_2 into useful chemicals or fuels, emphasizing sustainability [12]. Improving efficiency and net carbon benefits, understanding the mechanisms of reaction pathways, and scaling up the process industrial applications of CO_2 conversion under hydrothermal conditions are challenging. Integrated systems that capture CO_2 and convert it electrochemically have been developed to improve efficiency and scalability. These systems use renewable electricity to convert CO_2 into multi-carbon products, offering a pathway for industrial-scale implementation [13]. However, these systems are still in developmental stages and require substantial investment and improvement in efficiency to scale up to levels that would significantly impact global CO_2 emissions. As depicted in Fig. 1, four general steps are required for converting CO_2 to fuel products: 1) capturing CO_2 from stationary sources or directly from the air and then transporting the captured CO_2 to the refineries; 2) converting CO_2 to CO or CH_4, syngas, methanol, ethanol, and propanol using electrolysis or thermal catalysis; 3) convert syngas or other intermediate products via the Fisher-Tropsch process or oligomerization of ethylene, propene, C4+ olefins into hydrocarbons; and 4) fuel separation and finishing to produce fuel products and integrating the overall process and plant. Despite significant advancements in CO_2 conversion technologies, current studies and projects and their outcomes fall short of the global carbon reduction targets necessary to mitigate climate change effectively. Therefore, this paper investigates the economic and environmental impacts of two potential large-scale CO_2 conversion pathways to jet fuels, with one involving the Syngas direct Fisher-Tropsch process. The other one is converting methanol to olefins first and then olefin oligomerization to distillate using methanol as an intermediate.

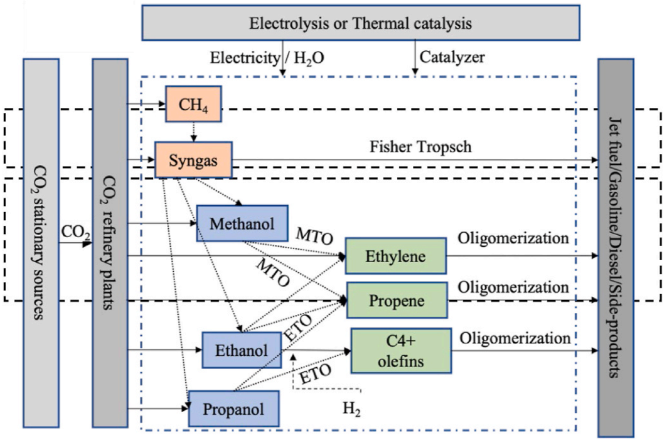


Fig. 1. Potential CO_2 conversion routes to produce fuels.

1.2. Techno-economic analysis for CO_2 conversion

Several prior studies have explored the techno-economic feasibility of different pathways for converting CO_2 into chemicals and fuels. A Gross-Margin model was developed to assess the techno-economic viability of various C_1-C_2 products produced through the electro-reduction of CO_2 [14]. This model optimized the performance benchmarks of different electro-reduction products, including carbon monoxide, formic acid, methanol, methane, ethanol, and ethylene [14]. In another investigation, a process mass and energy balance model in CHEMCAD evaluated the technological and economic feasibility of formic acid synthesis from CO_2 [4]. Calculations of molar flow rates were employed in a separate study to determine the capital investment, operating costs, and product revenue associated with CO_2 reduction to liquid products. Four potential routes, analyzed under various performance scenarios using a consistent model, assessed their techno-economic viability. The primary expense was the capital cost associated with the purchase and installation of the CO_2 electrolyzer [15]. Assessing the end-of-life net present value (NPV) of a generalized electrochemical CO_2 reduction (eCO_2R) plant under proposed performance targets revealed the profitability of chemicals and fuels production. NPVs indicated that electrochemical CO_2 reduction could be profitable, but improvements such as lower electricity costs and enhanced catalytic performance were needed to increase profits [16]. A techno-economic analysis was conducted by calculating the levelized cost of products from CO_2 reduction reactions to identify the most profitable products and the required performance targets [17]. Recently, a more intelligent, comprehensive, and fully automated process synthesis framework was developed to predict the levelized cost of chemicals derived from CO_2 conversion. This model explored 295 electrochemical coproduction combinations to identify profitable combinations of CO_2RR technology combined with value-added organic oxidation reactions (OORs) [18]. However, the techno-economic analysis for CO_2 conversion needs more comprehensive approaches that integrate real-world operational and market conditions, broader applicability and scalability analyses, and sensitivity analysis on key economic indicators. Additionally, there is a lack of exploration of fluctuating electricity prices, renewable energy integration, and validation of automated process synthesis frameworks against industrial-scale operations.

1.3. Supply chain network optimization

Geographically, the locations of CO_2 supply sites (stationary sources) and jet fuel end-use sites (airports) are not contiguous, which presents a challenge for establishing a supply chain network for the CO_2-to-Fuels conversion industry [19]. A strategic optimization of the supply chain network of CO_2 conversion is crucial for addressing this challenge by selecting the number, locations, and capacities of facilities at each stage of the supply chain. Numerous studies have focused on supply chain systems optimization for renewable fuel products. Various optimization techniques, such as linear programming (LP), mixed integer linear programming (MILP), and mixed integer nonlinear programming (MINLP), have been extensively utilized to develop technical and economic models for different carbon conversion technologies [20–23]. These models consider many factors, including the availability of feedstocks, the selection of conversion technologies, the locations of refineries, geographical diversity, infrastructure compatibility, demand distribution, and government incentives. For example, a multi-objective and multi-period MILP model that considered various conversion pathways and technologies was used to address the logistical challenges in a biomass-to-liquid system [24,25]. Although considerable attention has been given to supply chain systems for renewable fuel production, there are few quantitative models for optimizing the supply chain network design for CO_2 conversion to valuable jet fuel. To bridge all these research gaps, it is imperative to optimally integrate capture, transportation, conversion, and consumption activities to design efficient CO_2 conversion to fuel networks This paper builds a MILP model to optimize the supply chain network of CO_2 conversion to jet fuel with minimal total cost. The model determines the overall supply chain costs via different CO_2 conversion pathways, which include CO_2 capture costs, CO_2 and jet fuel transportation-related costs, refinery capital investment, and refinery operating costs. The originality of the developed optimization work includes 1) defining a large-scale CO_2 utilization process that includes carbon capture, conversion, and consumption (CCCC) scheme, 2) evaluating the techno-economic feasibility of FTS and MeOH conversion pathways and identifying the major cost drivers, and 3) calculating the carbon emissions from the conversion and transportation in the CO_2-to-Fuel process.

Therefore, the overall objective of this study is to evaluate the techno-economic feasibility and supply chain optimization of converting captured CO_2 from stationary sources into jet fuels and answers the following three questions:

1. Is it economically feasible and environmentally friendly to produce jet fuel via FTS and MeOH pathways in the United States?
2. What does the distribution network in the United States look like to supply jet fuels converted from the CO_2 captured at stationary sources?
3. How do electricity rates, feedstock prices, the CO_2 recycle percentage of the FTS pathway, and conversion rates impact the economic feasibility, environmental impacts, and network configuration for the CO_2 conversion to jet fuels?

2. Network design

This paper considers a three-stage CO_2-to-Fuels supply chain network, including I stationary CO_2 source sites (i as its index), J potential CO_2 conversion refineries (j as its index), and A large airports (a as its index) in the United States as jet fuel demand points. Each stationary source i has up to E_i tons of CO_2 to be captured annually at the cost of c_i^c per ton. CO_2 and H_2 are synthesized into jet fuels at refineries via S conversion pathways (s as its index). Each potential refinery j has an annual capacity to convert C_{sj} tons of CO_2 at the conversion rate of α^s and at the H_2 cost for processing one ton of CO_2 of c_j^h. Building and operating conversion capacity following pathway s at refinery j incurs c_{sj}^f annualized capital investment and c_{sj}^o operating cost per ton of CO_2. This study only considered transporting CO_2 by pipelines at the unit cost of c_{ij}^l (\$/t) from source i to refinery j. The transportation cost of jet fuel is performed by trucks and is c_{ja}^v (\$/t) from refinery j to airport a. The annual jet fuel demand at airport a is D_a tons. The average jet fuel sale price is p per ton. The model decides x_{ij} tons of captured CO_2 from source i transported to refinery j and y_{ja} tons of produced jet fuel from refinery j to airport a. The binary decision z_j^s represents the selection of conversion pathway s at potential refinery j. If no pathway is selected, it means no capacity is built at potential location j. The following list of notations is provided to facilitate the modeling.

2.1. (1) sets

$i \in I$: Index for stationary CO_2 source sites;
$j \in J$: Index for potential CO_2 conversion refineries;
$a \in A$: Index for airports;
$s \in S$: Index for CO_2 conversion pathways.

2.2. (2) parameters

c_i^c: Unit CO_2 capture cost at stationary source i;
α^s: CO_2 conversion rate via conversion pathway s;
c_j^h: Unit H_2 cost for processing one ton of CO_2 at potential refinery j;
c_{sj}^f: Annualized fixed capital investment of potential refinery j via conversion pathway s;
c_{sj}^o: Unit operating cost of potential refinery j via conversion pathway s;
c_{ij}^l: Unit cost for transporting CO_2 by pipelines from stationary source i to potential refinery j;
c_{ja}^v: Unite transportation cost of jet fuel is performed by trucks from potential refinery j to airport a;
E_i: Annual captured CO_2 from stationary source i;
C_{sj}: Annual production capacity of potential refinery j via conversion pathway s;
D_a: Annual jet fuel demand at airport a;
p: Average jet fuel sale price.

2.3. (3) variables

x_{ij}: Captured CO_2 from source i transported to potential refinery j;
y_{ja}: Produced jet fuel from potential refinery j to airport a;
z_j^s: Selection of conversion pathway s at potential refinery j.

The objective of the MILP model (1–6) is to minimize the net supply chain cost, which is the total costs minus the overall revenue. The total costs are comprised of five parts: CO_2 capture cost, H_2 purchase cost, CO_2 and jet fuel transportation cost, refinery capital investment, and refinery operating cost.

$$\begin{aligned}
\text{Minimize}\quad & \sum_{i\in I}\sum_{j\in J}\left(c_i^c + c_j^h + c_{ij}^l\right)x_{ij} + \sum_{i\in I}\sum_{j\in J}\sum_{s\in S}c_{sj}^o x_{ij} + && (1)\\
& \sum_{j\in J}\sum_{s\in S}c_{sj}^f z_j^s + \sum_{j\in J}\sum_{a\in A}\left(c_{ja}^v - p\right)y_{ja} && \\
\text{s.t.}\quad & \sum_{i\in I}\sum_{s\in S}\alpha^s x_{ij} = \sum_{a\in A}y_{ja} \qquad \forall j \in J && (2)\\
& \sum_{i\in I}x_{ij} \le \sum_{s\in S}C_{sj}z_j^s \qquad \forall j \in J && (3)\\
& \sum_{j\in J}x_{ij} \le E_i \qquad \forall i \in I && (4)\\
& \sum_{j\in J}y_{ja} \le D_a \qquad \forall a \in A && (5)\\
& \sum_{s\in S}z_j^s \le 1 \qquad \forall j \in J && (6)\\
& x_{ij}, y_{ja} \ge 0;\ z_j^s \in \{0,1\}\ldots &&
\end{aligned}$$

Objective function (1) minimizes the total costs of converting CO_2 to jet fuel of the entire supply chain. Constraint set (2) maintains conversion balance at each facility j. Constraint set (3) enforces refineries' conversion capacity. Constraint set (4) makes sure that the amount of captured CO_2 does not exceed the available CO_2 emissions at sources. Constraint set (5) ensures the airports' demand bounds the produced jet fuel shipped to an airport. Constraint set (6) guarantees that each potential conversion facility only uses at most one conversion pathway.

3. System boundary and data description

3.1. CO_2-CO-FTS-fuel and CO_2-Methanol-Fuel routes

The Fischer-Tropsch synthesis (FTS) process converts a mixture of carbon monoxide (CO) and hydrogen (H_2) into liquid hydrocarbons, which can be futher refined into synthetic jet fuels. Notably, synthetic jet fuel produced via the FTS process has been approved for commercial aviation use in a blend of up to 50 % with conventional jet fuel [26]. This approval underscores the potential of FTS-based synthetic jet fuel to serve as a viable and sustainable alternative for the aviation industry. The process begins with the electrocatalytic reduction of carbon dioxide (CO_2) with water (H_2O) to produce carbon monoxide (CO). Then, CO is then combined with hydrogen (H_2) and converted into synthetic fuels through the Fischer-Tropsch process. The CO_2-CO-FTS system process is depicted in Fig. 2 and involves the following four steps:

1) Electrocatalytic Reduction. CO_2 is captured from industrial sources or directly from the air and fed to an electrolyzer. In the presence of water (H_2O) and an electrocatalyst, CO_2 undergoes a reduction reaction to form carbon monoxide (CO) and hydroxideions (OH^-) with the following reaction:

$$CO_2 + H_2O + 2e^- \rightarrow CO + 2OH^-; \tag{7}$$

2) Syngas Composition. The resultant CO from the above reactions is combined with additional H_2 to form synthesis gas (syngas), a mixture of CO and H_2.
3) Fischer-Tropsch Synthesis (FTS). The syngas is introduced into a reactor containing a Fischer-Tropsch catalyst (typically iron or cobalt). Under specific conditions of temperature and pressure, the catalyst facilitates the polymerization of CO and H_2 into long-chain hydrocarbons. 85.8 % unreacted CO_2 will be recycled into the previous step and electrolyzed into CO.
4) Hydrocarbon Separation. The mixture of hydrocarbons produced in the FTS reactor includes a variety of products such as paraffins, olefins, naphtha, and diesel. These products are then separated through distillation and other refining processes to obtain the desired jet fuel [27,28].

The CO_2-Methanol-Fuel (MeOH) route involves the converiosn of captured CO_2 into methanol, which is then transformed into liquid hydrocarbon fuels, including synthetic jet fuel. This process offers a sustainable pathway to produce renewable jet fuel, leveraging methanol's versatility as a platform chemical. ExxonMobil has also exhibited the conversion of methanol into middle distillate fuels such as diesel and kerosene. The CO_2-Methanol-Fuel (MeOH) route is illustrated in Fig. 3 and involves the following steps:

1) CO_2 Conversion to Methanol. Currently, commercial methanol production relies on synthesis gas containing CO and H_2. Several methods can produce methanol from CO_2, including direct thermocatalytic conversion, direct electrocatalytic conversion, direct photocatalytic conversion, and hybrid approaches. Direct CO_2 conversion to methanol follows the following reaction:

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O. \tag{8}$$

2) Methanol to Hydrocarbons. Methanol is first converted into light olefins (such as ethylene and propylene) over zeolite catalysts.
3) Production of Synthetic Jet Fuel. The light olefins are then oligomerized (combined to form longer chains) and hydrotreated to produce liquid hydrocarbons, including synthetic jet fuel. This process involves combining smaller hydrocarbon molecules into longer ones and refining them to meet jet fuel specifications.

3.2. *Techno-economic performance of FTS and MeOH*

Table 1 shows the annualized capital investment, unit operating cost, and conversion rate of the FTS and MeOH pathways and the CO_2 recycle rate at the FTS pathway. The reaction equations (7) and (8) of the two pathways show that H_2 is an important feedstock to produce hydrocarbon fuels via reacting with CO_2. A recent review discussed the status of water electrolysis technologies for H_2 production [29]. The leading technologies are alkaline electrolysis (AEL), proton exchange membrane electrolysis (PEMEL), and solid oxide electrolyzer cells (SOEC). AEL is the most mature technology and currently has the lowest investment and maintenance costs among these three technologies, which have been commercially available for over a century. From the existing studies, the H_2 consuming is 0.27 and 0.44 kgH_2 per kg_{fuel} in the FTS and MeOH route, respectively [30]. The study assumes a hydrogen price range based on current and projected market conditions, which fluctuates from $0.8/kg to $5.0/kg [31]. However, this assumption may not accurately reflect future market volatility or regional price differences.

In general, CO_2 used in synthesis can be obtained from stationary sources with a high CO_2 partial pressure, such as power plants, or directly from the air using direct air capture (DAC) technologies. DAC requires significantly higher energy inputs and involves processing larger gas volumes compared with capturing CO_2 from stationary sources. Therefore, this study only considered capturing CO_2 from power plants. The primary CO_2 capture technologies from stationary sources are absorption and adsorption. From an existing techno-economic analysis, one ton of CO_2 can be converted to 0.46 tons of FT fuel (the summation of 26 % naphtha, 47 % jet fuel, and 27 % diesel) [32]. Considering the recycling of unreacted CO_2 in the FTS pathway, the utilized CO_2 fraction is calculated by dividing the converted CO_2 by the product of one minus the unused CO_2 fraction and the recycled CO_2. Generally, it is estimated that the production of 1 MJ (50 g) of methanol requires 83 g of CO. In an ideal process, 2,260g of methanol would be needed to produce 1000g of jet fuel. Consequently, 1 kg of CO_2 can yield 0.265 kg of jet fuel via the MeOH pathway. The co-products in the MeOH pathway include 0.212 kg of diesel, 0.053 kg of gasoline, and 0.053 kg of liquefied petroleum gas [33]. The estimated cost of capturing CO_2 from different types of power plants ranges from $35 to $112 per ton [34]. The conversion rates and recycle percentages are based on laboratory-scale experiments as mentioned before, which may not translate directly to industrial-scale operations. There is a risk of overestimating the efficiency and performance of these processes when scaled up, potentially leading to optimistic economic feasibility projections.

We assumed the potential refineries can produce 100 kt of jet fuel per year requires 600 MW_e of installed electrolyzer production capacity, with a 30-year lifetime and 365-day operating time per year for both FTS and MeOH pathways. Electricity stands as the primary contributor to the annual operational costs for electrolyzers and other equipment in the entire process. The FTS and MeOH pathways require 279 to 838 kWh and 828 to 1656 kWh of electricity, respectively, to produce one ton of jet fuel [35]. The U.S. grid price of $0.06 per kWh was first applied to

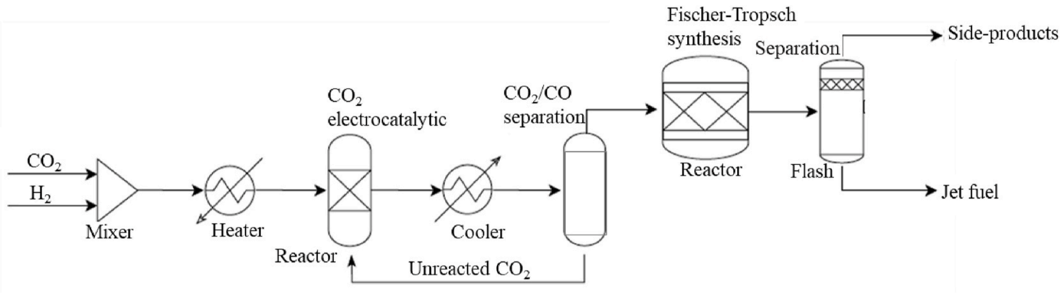


Fig. 2. Simplified CO_2-CO-FTS process.

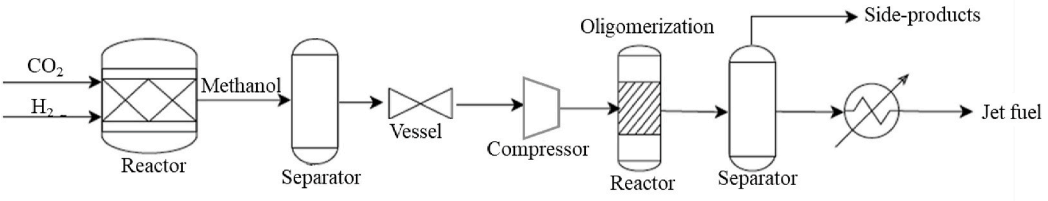


Fig. 3. Simplified CO_2-Methanol-Fuel process.

Table 1
Characteristic of FTS and MeOH pathways.

	FTS	MeOH
Annualized capital investment, $/yr	9,125,625.0	9,653,250.0
Unit operating cost, $/t*		
Synthesis and conditioning	2400.0	2500.0
Electricity	16.7–50.3	49.0–99.4
Conversion rate of pathways, %	21.6 %	26.5 %
CO_2 recycle rate of FTS pathway, %	85.8 %	–

* $/t means US Dollars per ton of produced jet fuel.

both pathways in this study, with a subsequent analysis considering varying electricity prices across states. In addition, the other operating cost for synthesis and conditioning are $2400 and $2500 for the FTS and MeOH pathways, respectively, to produce one ton of jet fuel [36]. As the unreacted CO_2 will be recycled for the FTS pathway, the production time for this pathway is calculated as one divided by one minus the unused CO_2 fraction times the recycled CO_2 fraction as shown in equation (9). The unit refinery operations costs for the FTS pathway are the unit refinery operations cost ($/t/yr) without considering recycling, multiplied by the production time. The total one-time capital investment, yearly operating costs, and the discounted cash flow of the FTS and MeOH pathways were evaluated. Four levels of capital investment have been considered: Bare Erected Cost (BEC), Engineering, Procurement and Construction Cost (EPCC), Total Plant Cost (TPC), and Total Overnight Capital (TOC). The one-time annualized capital investments are $9,125,625 for the FTS pathway and $9,653,250 million for the MeOH pathway, with an annual interest rate of 10 % for each [36].

$$Production\_time_{FTS} = 1 \Big/ \left(1 - CO_{2unsued} \times CO_{2recycled}\right) \tag{9}$$

This study conducts a techno-economic analysis for the United States, dividing the contiguous 48 states into 407 grids based on the U.S. 4-Digit Maidenhead Grid Squares system [37]. Each 2° by 1° grid approximately represents an area of 100 by 70 miles. The assumption is made that each grid could potentially host a refinery. Additionally, each stationary CO_2 emission source is considered a potential refinery location. Consequently, the study considers 1337 stationary sources, 1746 potential refinery locations, and the 47 most heavily trafficked airports, as depicted in Fig. 4. The dot size at a source or airport is proportional to the available CO_2 or jet fuel demand, respectively. Two CO_2 conversion pathways for potential refineries are examined in the analysis, resulting in a total of 219,433,788 scenarios related to CO_2-to-Fuels conversion within the framework of supply chain network topologies. To enhance solver runtime efficiency, the United States is divided into five regions: Southeast, Northeast, Midwest, West, and Southwest. The MILP model (1–6) was solved for each region to obtain the optimal supply chain network. The resulting solution includes: 1) the selection of stationary sources and refineries, along with their respective annual volumes; 2) the choice of the conversion pathway for each selected refinery; 3) the amount of CO_2 captured at each source and converted at each selected refinery; and 4) the distribution of jet fuel from refineries to airports.

The total network cost is the summation of CO_2 capture cost, H_2 purchase cost, CO_2 and fuels transportation cost, annualized refinery capital investment, and refinery operating cost, subtracted by the total revenue from selling jet fuel and co-products. Table 2 provides data sources for all required parameters in the model and analysis. A stepwise optimization approach was employed to calculate the minimum levelized cost of CO_2 transport by pipeline over a designed lifetime of 25 years. This calculation considered different pipeline nominal diameters, wall thicknesses, operational pressures, and the number of boosting pump stations. The levelized cost encompasses both capital investment and operating costs, resulting in a range of 8.26 $/t$CO_2$ – 8.72 $/t$CO_2$. This cost estimate corresponds to a temperature range from −20 °C to 17 °C for a pipeline with diameters ranging from 0.4064 m to 0.4572 m, designed for a length of 150 km and a CO_2 mass flow rate of 252 kg/s [38]. The total transportation cost for jet fuel by trucks is determined by the unit variable transportation cost, the quantity of jet fuel being transported, and the transportation distance [39]. This study assumes a

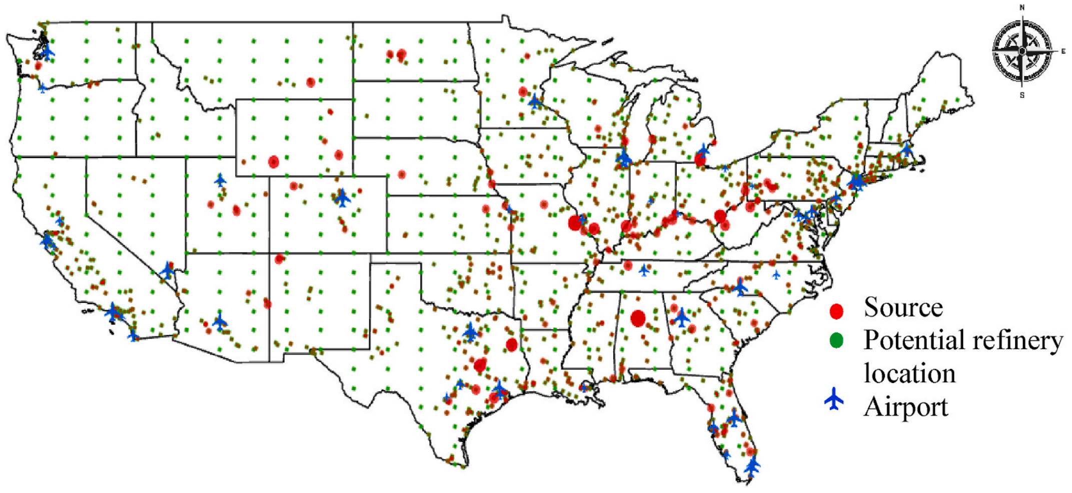


Fig. 4. Distribution of stationary sources, potential refineries, and major airports.

Table 2
Data values and sources for all parameters.

Parameters	Values	Sources	Parameters		Sources
Costs			**Others**		
Unit pipeline cost, \$/t/mile	8.26–8.72	[38]	U.S. stationary CO_2 source locations	GitHub	[19]
Unit variable truck cost, \$/t/mile	0.9	[39]	U.S. stationary CO_2 source emissions, t/yr	GitHub	[19]
Unit fixed truck cost, \$/t	24	[39]	Potential refinery locations	GitHub	[37]
Jet fuel sale price per ton, \$/t	732.5	[40]	Top 47 busiest airport locations in the U.S.	GitHub	[41]
Unit CO_2 capture cost, \$/t	35–112	[34]	Annul jet fuel demands, Mt/yr	GitHub	[36]
Annualized refinery capital cost, \$	Table 1	[36]	Electricity price by states, \$/kWh	GitHub	[42]
Unit refinery operational cost, \$/t	Table 1	[35]	Conversion rate of pathways	Table 1	[32,33]
Unit H_2 price, \$/t	800–5000	[31]	CO_2 recycle rate of FTS pathway	Table 1	[32]

variable transportation cost of 0.9\$/t/mile and a fixed transportation cost of 24.0 \$/t, which remains independent of distance. The distance between two points is approximated by the straight-line distance derived from their latitude and longitude coordinates. Assuming a truck with a 120-gallon fuel tank can travel approximately 600 miles at a fuel consumption rate of 6 mpg and considering government regulations limiting a truck driver's maximum travel distance, we restrict that potential refineries should be located within 300 miles of airports. Refinery costs encompass one-time capital investment and operating costs, including expenses for feedstock purchase, equipment installation, electricity usage, management, and maintenance. Revenue is generated by selling jet fuel and side products to airports and other customers. The market price of jet fuel in the U.S. stood at 732.5 \$/t in 2023 [40]. For more information, please see the values of these parameters following the GitHub link in Data Availability.

4. Results

4.1. Resulting network

Under the current cost structure, both paths cannot realize profitability. To be futuristic, we assumed the hydrogen price at \$1000/t and reduced the operating cost to its 5 %. The map in Fig. 5(a) demonstrates the resulting distribution network map under varying electricity rates across states. The FTS pathway is implemented at all refineries. All 14 selected refineries are strategically situated in states characterized by lower electricity rates and proximate to the 108 selected stationary sources, obviating the necessity for new pipelines to transport the captured CO_2. The distances between refineries and airports are meticulously maintained within a 300-mile radius.

In addition, we explored the network configuration under the assumption of uniform electricity prices (\$0.06/kWh) across all states. Fig. 5(b) and (c) provide a comparative analysis of the network maps for four airports: Harry Reid International Airport (LAS), Los Angeles International Airport (LAX), John Wayne Airport (SNA), San Diego International Airport (SAN), and Phoenix Sky Harbor International Airport (PHX). The depicted maps reveal that under different electricity rates for all states, the cost-optimal supply chain analysis advocates to build refinery in lower electricity location. Given the same electricity rate for the whole nation, the refineries will be strategically located in proximity to areas exhibiting higher demand for jet fuel.

To facilitate a comparative assessment of both the CO_2 conversion efficiency and economic viability of the FTS and MeOH pathways, we conducted separate executions of the optimization model for each pathway alone, considering different electricity prices by state. The outcomes reveal that on the condition of \$1000/t H_2 price and 5 % of the operating cost, the MeOH pathway is still not economically feasible. However, the overall annual profit of the FTS pathway is \$8 billion with a cost of \$73 billion and the revenue generated from selling jet fuel and side-products at \$81 billion. The profit of the FTS pathway is. The FTS pathway could potentially convert 116,724,796 tons of CO_2 into 46,938,776 tons of jet fuels per year, which 100 % meet the jet fuel demand in the selected airports. Notably, the pipeline length is 1809 miles, and the one-way truck transportation distance spans 4493 miles. The comparison indicates that the costs associated with CO_2 capture, H_2 purchase, refinery capital, and refinery operations are lower for the FTS pathway than the MeOH pathway. In addition, the difference is caused by the recycling of CO_2 within the FTS pathway, with the expense of H_2 purchase and the operating of the refinery being the predominant contributor to the total cost. Although the overall MeOH pathway is not economically feasible under the assumed cost structure, the profit of selling side-products in the MeOH pathway is higher than the FTS pathway. If its conversion rate could be improved, the production of jet fuel through MeOH would be profitable. Subsection 4.2 provides the sensitivity analysis of the conversion rate of the MeOH pathway.

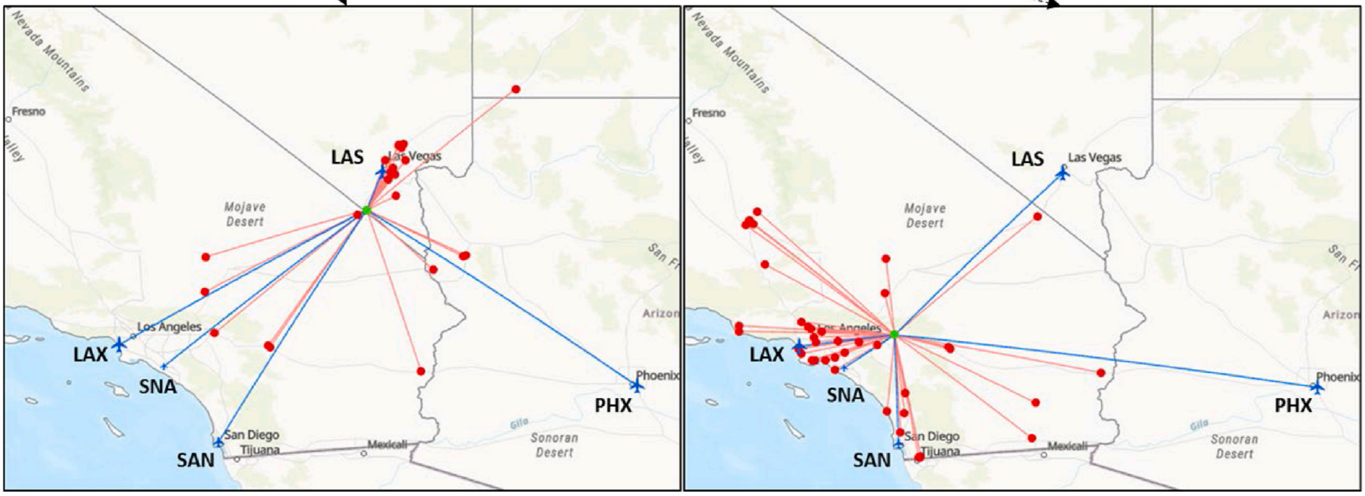
The life cycle assessment was modeled in OpenLCA using NETL CO_2U LCA [43] and exiobase 2.2 [44] open-source databases to assess the environmental impact of the integrated CO_2 conversion to jet fuel transportation and production process. A comparison of the global warming potential of jet fuel produced from the optimal, FTS-only, and MeOH-only pathway was conducted. The system boundaries are defined according to the cradle-to-gate approach. One kg of produced jet fuel is considered a functional unit, and TRACI 2.1 was used to calculate an impact assessment method [44]. The life cycle inventory data were created based on the generated mass balance.

Without considering the economic feasibility, both FTS and MeOH pathways exhibit net negative CO_2 emissions. Specifically, the FTS pathway results in 11,249,866 tons of CO_2 emissions during production and transportation on the condition of 1000\$/t H_2 price and 5 % of the operating cost, while to produce the same amount of jet fuel, the MeOH pathway scenario emits 3,510,806 tons of CO_2 per year. The total CO_2 capture amounts per year are 116,724,796 tons for the FTS pathway scenario and 95,229,814 tons for the MeOH pathway scenario. Net carbon emissions per year are computed as the emissions during production and transportation minus the used CO_2, which are −88,783,284 tons for the FTS pathway scenario, and −6,497,200 tons for the MeOH pathway scenario. The optimal nationwide CO_2-to-Fuels supply chain network is presented in Table 3.

4.2. Sensitivity analysis

The network results indicate that the major cost contributors of CO_2-to-Fuels come from hydrogen usage and operating expense. From the description of the CO_2-CO-FTS-Fuel and CO_2-Methanol-Fuel routes in Subsection 3.1, it is evident that two additional significant parameters are the CO_2 recycle percentage of the FTS pathway and the CO_2 conversion rate. We conducted a sensitivity analysis, exploring the impact of the unit H_2 price, unit refinery operating cost, the CO_2 recycle percentage of the FTS pathway and the CO_2 conversion rate on total profit, utilized CO_2, and produced jet fuel. The DOE's Hydrogen and Fuel Cell Technologies Office aims to develop technologies that can produce hydrogen at \$2/kg by 2026 and \$1/kg by 2031 through net-zero-carbon pathways, supporting the Hydrogen Energy Earth shot goal of reducing the cost of clean hydrogen by 80 % to \$1 per kilogram within a decade [45]. The range of unit operating costs was determined based on

(a) Nationwide CO_2-to-jet fuel supply chain network



(b) Under different electricity prices by states

(c) Under the same electricity price in the nation

Fig. 5. (a) the nationwide CO_2-to-jet fuel supply chain network in the U.S. based on the electricity prices by state in 2022, 1000$/t H_2 price and 5 % of the operating cost. (b) and (c) are regional CO_2-to-jet fuel supply chain network map for LAX, SNA, SAN, LAS and PHX airports under average electricity rates by state and same electricity rate across the states in 2022, $1000/t H_2 price and 5 % operating cost.

experimental testing and analysis. Fig. 6 is the optimal total profits when the H_2 price ranges from $600/t to $1300/t and the unit operating costs are between 4 % and 8 % of the current cost, which is possible when the conversion happens during the off-peak time when the penetration rate of renewable energy further increases. Fig. 6 shows that a H_2 price below $900/t will make the conversion idea profitable.

Fig. 7 is the heatmap of the profits under different H_2 prices and unit operating costs of both pathways. The result shows that the MeOH pathway requires much lower H_2 price and unit operating cost to be economically feasible than the FTS pathway. Click or tap here to enter text. To make production profitable, the unit operating cost should be reduced to 6 % of the current rate via the FTS pathway. For the MeOH pathway, the H_2 price should be further reduced to $700/t to realize profit. Fig. 8 is the utilized CO_2 and produced jet fuel under different H_2 price and operating cost under the optimal solution considering both pathways. The result indicates that, the utilized CO_2 and produced jet fuel start to increase when the H_2 price is below $1000/ton and the operating cost is reduced to 6 % of the current level.

As previously discussed in section 3.1, the current CO_2 recycle percentage stands at 86 %. To explore the impacts of varying this percentage, we tested five scenarios with 10 % intervals. Fig. 9 depicts the outcomes of a sensitivity analysis examining the CO_2 recycle percentage ranging from 56 % to 96 %, with 86 % serving as the baseline. The result reveals a clear relationship between the CO_2 recycle percentage and total costs. Our findings indicate that when the CO_2 recycle percentage is equal to or less than 56 %, the CO_2-to-Fuels conversion process becomes infeasible. Beyond the 86 % threshold, all of the costs and utilized CO_2 will decrease while the system can fulfill the total jet fuel demand at the selected airports. The refinery capital costs remain constant across all observed variations in CO_2 recycle percentages.

As illustrated in Fig. 10, the optimal levels of captured CO_2, utilized CO_2, and produced jet fuel, under both relatively low and high H_2 prices and operating costs, are contingent upon varying CO_2 conversion rates ranging from 30 % to 90 %. The current CO_2 conversion rate ranges from 22 % to 26 %. To observe more dramatic changes, we increased the CO_2 conversion rate beyond this range in our analysis. Fig. 10(a) shows the optimal total profit and captured CO_2 under the lower cost scenario ($100/t for the H_2 price and 3 % of the operating cost). In this scenario,

Table 3

Nationwide CO_2-to-Fuels supply chain network results of optimal pathways under the conditions of an 85.8 % CO_2 recycle rate for FTS pathways, a $1000 per ton unit H_2 price, and 5 % of the operating cost.

Costs	Unit, $/t	Total, $/yr
CO_2 capture	183	8,579,272,478
H_2 purchase	709	33,266,566,750
Refinery capital	3	127,758,750
Refinery operations	569	26,689,190,364
Pipeline	4	182,057,768
Truck transportation	75	3,537,900,995
Total cost	1542	72,382,747,105
Revenue, $/yr	–	
Jet fuel	–	34,382,653,061
Naphtha	–	16,213,252,280
Diesel	–	29,939,049,066
Gasoline	–	0
Liquefied petroleum gas	–	0
Total revenue	–	80,534,954,407
Profit, $/yr	–	8,152,207,302
Transportation, mile	–	
Pipeline length	–	1809
Truck travel distance	–	4493
CO_2, ton	–	
Captured CO_2	–	116,724,796
Used CO_2	–	100,033,150
Unused CO_2	–	16,691,646
Emissions during production and transportation	–	11,249,866
Net CO_2 emissions	–	−88,783,284
Jet fuel, ton/yr	–	46,938,776
Jet fuel demand meet, %	–	100 %

all demands are met, and the utilized CO_2 and produced jet fuel amount to 99,870 kt and 46,939 kt, respectively. Of course, the captured CO_2 decreases with increasing conversion rates. Within the range of 30 %–70 % conversion rates, the FTS pathway dominates the MeOH pathway at all selected refineries, whereas beyond an 80 % conversion rate, the MeOH pathway prevails. This can be attributed to the inherent CO_2 recycling mechanism within the FTS pathway, resulting in a higher final CO_2 conversion rate compared to the MeOH pathway. When the conversion rate is very high, the recycling advantage diminishes. However, despite the FTS pathway's advantage in profit generation in most cases, the MeOH pathway demonstrates higher revenue due to its capacity to produce additional side-products. Consequently, while the MeOH pathway may initially appear economically unfeasible at lower CO_2 conversion rates, an increase in the conversion rate renders this pathway financially viable. Conversely, as depicted in Fig. 10(b), under higher costs, the FTS pathway emerges as the preferred choice for all refineries regardless of fluctuations in the CO_2 conversion rate. It is noteworthy that under a 30 % CO_2 conversion rate, the demand for jet fuel cannot be fully met.

A Monte Carlo simulation approach [46] is used to evaluate how uncertainties in four key parameters (unit CO_2 capture costs, unit H_2 costs, CO_2 recycle rate of FTS pathway, and conversion rates impact the total cost, total profit, and total net carbon emissions of the system. For each parameter, a normal distribution was assumed, with a standard deviation set to 10 % of the mean to introduce variability. The total cost, total profit, and total net carbon emissions are calculated by running the model under different random samples of these parameters across 100 Monte Carlo simulations as shown in Fig. 11. This plot highlights the range, median, and interquartile range (IQR). The result indicates that the total cost exhibits the most significant variation among the three metrics analyzed. The total profit demonstrates less variability, as reflected by a narrower IQR. The total net carbon emissions display a moderate range of variation. This suggests a moderate amount of uncertainty in the carbon emission outcomes, though it is less variable than the total cost but more than the total profit.

5. Discussion

Our study underscores the optimal network design for CO_2 conversion to jet fuel considering both cost-effectiveness and environmental concerns. The comparison of this study with previous in economic viability, supply chain optimization, and environmental benefits aspects are discussed in Table 4.

The study highlights that achieving a hydrogen price below $900/t is critical for making CO_2 conversion processes economically viable. The findings suggest that with current technological advancements and projected cost reductions make scaling up these processes to industrial levels is achievable. This also underscores the importance of policy measures that support the development and deployment of cost-effective hydrogen production technologies. The electricity rate constitutes a substantial component of the operational expenses incurred by refineries, which implies the importance of using renewable energy during the conversion, especially during the energy surplus period. Consequently, optimal refinery sitting favors locations with lower electricity rates to mitigate operational costs associated with refinery activities. Regions with abundant renewable energy resources and lower electricity prices, such as certain parts of the United States and Europe, may find it more economically viable to conduct conversion. As the transition to renewable electricity progresses, an anticipated decrease in electricity rates from $0.060/kWh to $0.029 kWh is expected to result in a significant reduction in refinery operations costs [47]. This shift will enable the establishment of refineries closer to airports, enhance transportation efficiency, and potentially reduce overall transportation

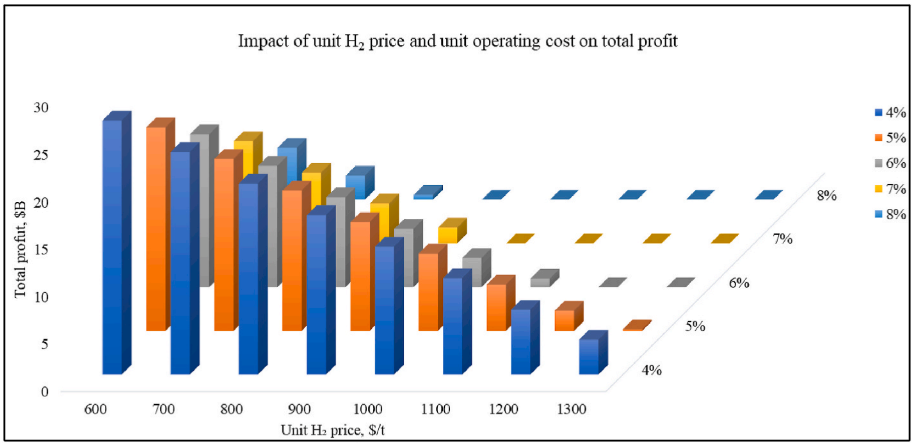


Fig. 6. Sensitivity analysis: Impact of unit H_2 price and unit CO_2 capture cost on profits.

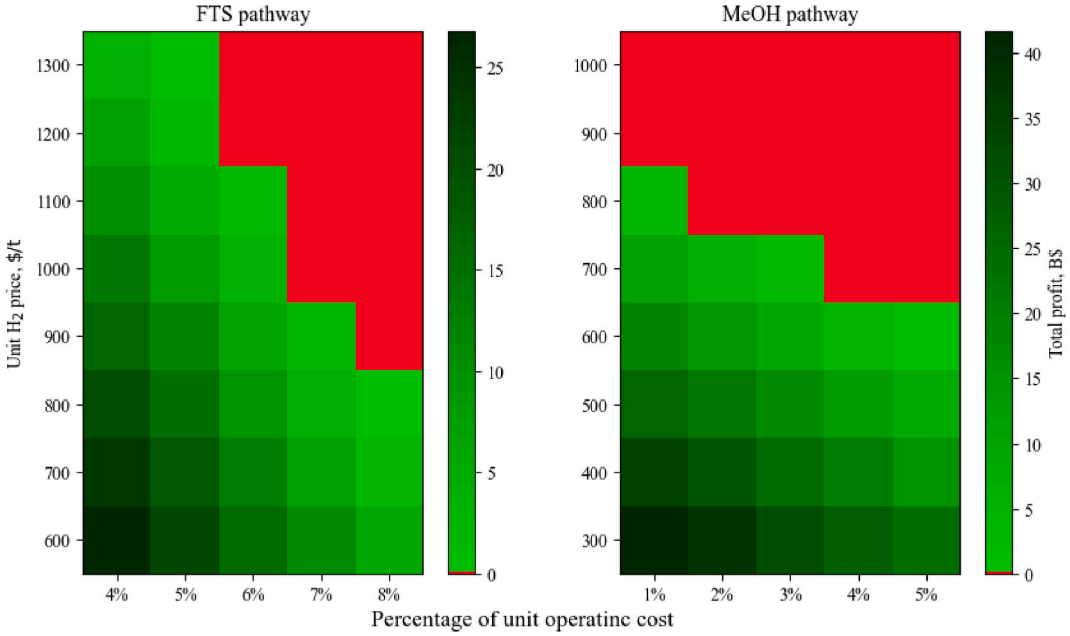


Fig. 7. Heatmaps of the CO_2 operating cost and H_2 purchase cost on profits of FTS pathway and MeOH pathway.

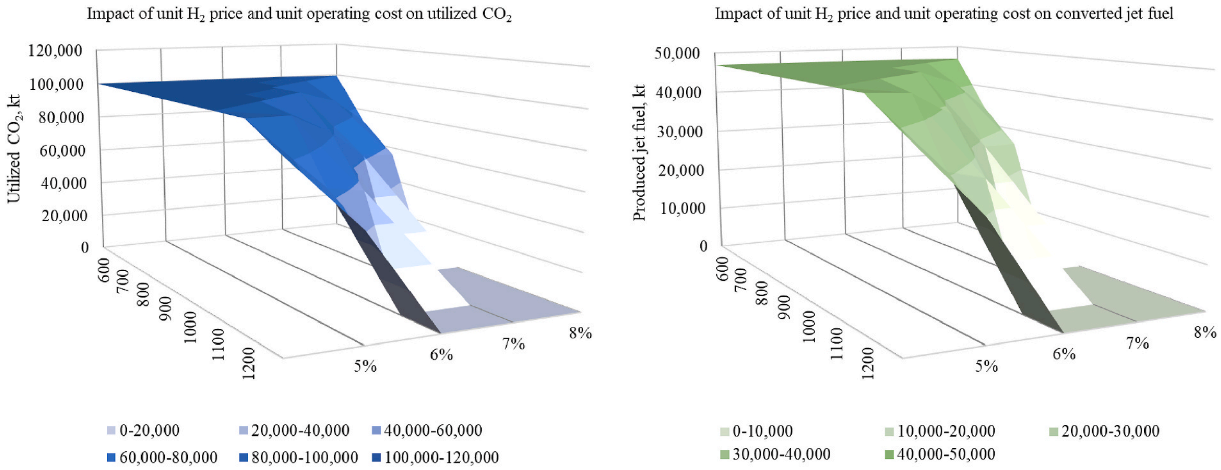


Fig. 8. Sensitivity analysis: Impact of H_2 price and CO_2 capture cost on utilized CO_2 and produced jet fuel.

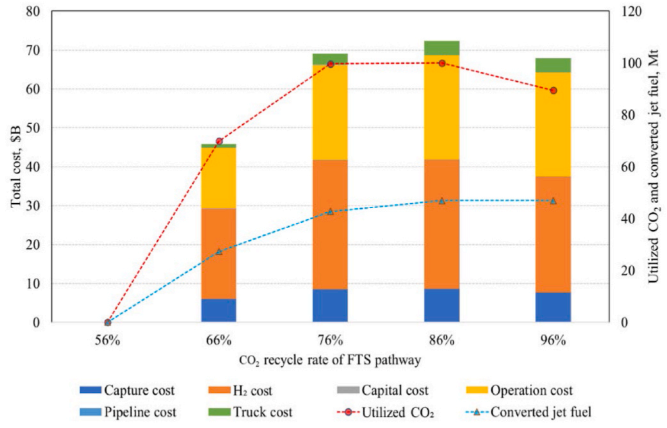
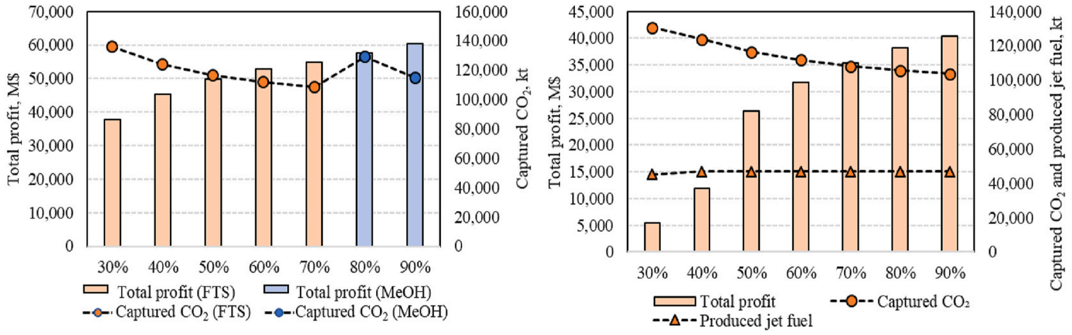


Fig. 9. Sensitivity analysis: Impact of the CO_2 recycle percentage of the FTS pathway on costs and profits, 56 %, 66 %,76 %,86 % (base case), and 96 % CO_2 recycled.

expenses and emissions. The recycling percentage within the FTS pathway plays a pivotal role in determining the applied conversion pathway at refineries. Since CO_2 will be recycled of the FTS pathway, the final conversion rate of this pathway is higher than the MeOH pathway. Therefore, the FTS pathway dominates all the refineries at the base scenarios. Our analysis reveals an inverse relationship between the CO_2-to-Fuels conversion rate and costs associated with CO_2 capture, H_2 purchase, annualized refinery capital investment, refinery operations, and fuel transportation. Thus, increasing the conversion rate is deemed crucial for enhancing the economic viability of the CO_2-to-Fuels technologies, especially for MeOH pathway. This finding emphasizes the need for continued research and development in CO_2 conversion technologies to improve efficiency. Pipeline construction costs significantly influence refinery location decisions due to substantial initial investments in land use and labor. In our study, the proximity of selected sources to the refineries results in significant cost savings.

The CO_2-to-Fuels through the FTS and MeOH pathways holds significant environmental potential by effectively reducing carbon emissions from stationary power plants and contributing to climate change mitigation. Both the FTS and MeOH pathways exhibit a noteworthy



(a) The optimal results under lower costs

(b) The optimal results under higher costs

Fig. 10. Impact of CO_2 conversion rate on total profit, utilized CO_2, and produced jet fuel of the optimal pathway. (a) the optimal total profit and captured CO_2 under \$100/t of H_2 price and 3 % of operating cost. (b) the optimal total profit, captured CO_2 and produced jet fuel under \$500/t of H_2 price and 5 % of the unit operating cost.

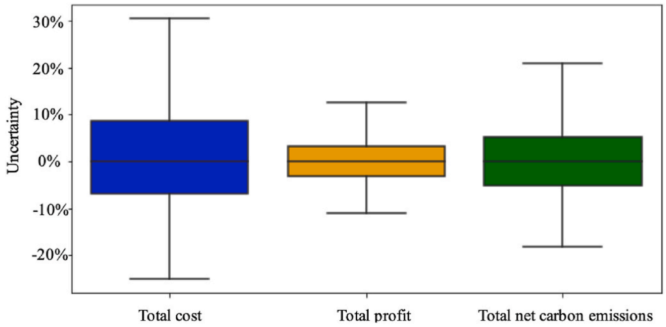


Fig. 11. Distribution of the total cost, total profit, and total net carbon emissions.

characteristic of being CO_2 emission negative. This unique feature allows for the continued utilization of high-value jet fuel without contributing excess energy and emissions from transportation-related activities. Utilizing renewable energy sources for hydrogen production and CO_2 conversion can further enhance the environmental benefits by reducing the reliance on fossil fuels and decreasing the overall carbon footprint of the process. While there are some potential trade-offs the environmental implications of the CO_2 conversion process. Achieving net negative CO_2 emissions through these conversion processes requires substantial energy input. If this energy is not sourced from renewables, the benefits of CO_2 sequestration might be offset by the emissions from energy production. Besides, the processes require significant water input, which can be a concern in arid regions. Balancing the benefits of CO_2 reduction with sustainable water use is crucial.

Supportive policies can help internalize the environmental cost of carbon emissions, making CO_2 conversion economically attractive. Government grants, tax credits, and funding for research and development can accelerate technological advancements in CO_2 conversion and hydrogen production and reduce the economic barriers to innovation and commercialization. Implementing carbon pricing mechanisms and emissions trading systems can incentivize industries to adopt CO_2 conversion technologies. Currently, DOE is establishing regional Hydrogen Hubs across the U.S., which are designed to integrate hydrogen production, storage, distribution, and end-use in a coordinated manner [52]. These hubs will play a pivotal role in scaling up the infrastructure needed for hydrogen production from CO_2, aligning with the goals of this study. The U.S. federal government offers the 45Q tax credit for carbon capture and sequestration, incentivizing companies to invest in technologies that capture and utilize CO_2 [53]. This policy directly supports the kind of CO_2 conversion into jet fuels explored in our study, making such technologies more attractive for commercial adoption. In summary, the combined application of techno-economic analysis and network design for CO_2 conversion to fuels represents tools for a comprehensive evaluation of feasibility and viability.

Table 4
Comparison with previous studies.

	Economic Viability	Supply Chain Optimization	Environmental Benefits
This Study	Hydrogen prices below \$900/t and reducing operating costs to 5%–6% of current levels are critical. The FTS pathway is more viable under current conditions.	MILP model optimizes the supply chain network, considering factors like CO_2 capture costs, hydrogen prices, electricity rates, and geographic distribution.	Potential for net negative CO_2 emissions in both FTS and MeOH pathways. Significant environmental benefits with renewable energy use.
[48]	The levelized cost of product CO (LCOC) of the cCO_2RR process is 3.5 times higher than that of the CO_2RR process, indicating low economic feasibility currently, but with potential for future cost reductions.	–	Life cycle assessment shows that using renewable electricity can result in a much more positive environmental impact for the cCO_2RR process compared to the CO_2RR process, even at current technological performance levels
[49]	Integration of highly efficient solid oxide electrolysis cells (SOECs) provides a low-cost solution for high syngas production rates at low cell degradation, significantly influencing economic viability.	–	The overall energy efficiency is 67 % with stable operation for 4000 h, emphasizing the importance of energy management and renewable energy integration.
[50]	The cost-effectiveness of CO_2 conversion to jet fuels highly depends on strategic locations and infrastructure.	The role of location and infrastructure in minimizing costs is important.	–
[51]	CO2-to-SAF via low/high-temperature electrolysis (LTE) is cost competitive, which is sensitive to feedstock costs and economies of scale.	Traffic forecasts and fuel price projections are integrated to optimize the supply chain for sustainable aviation fuels.	The integration with renewable energy sources has potential for substantial carbon footprint reduction.

6. Conclusion

This study proposed a detailed techno-economic analysis and mixed-integer linear programming model for the optimal design and operation of the CO_2 conversion to jet fuel supply chain in the United States. The analyses result in the following three major findings. 1) The Fischer-Tropsch synthesis (FTS) pathway is economically viable under current hydrogen prices and reduced operating costs, achieving a potential annual profit of $8 billion for the whole United States. However, the methanol (MeOH) pathway requires further improvements in conversion rates and hydrogen cost reductions to become feasible. 2) The sensitivity analysis reveals that hydrogen price and electricity costs are critical determinants of economic feasibility. Higher CO_2 recycle percentages and conversion rates significantly enhance the economic and environmental performance of CO_2 conversion pathways. 3) Both the FTS and MeOH pathways can achieve net negative CO_2 emissions, contributing to global carbon reduction goals and demonstrating the potential for these technologies to mitigate climate change. The findings of this study underscore the potential for large-scale implementation of CO_2 conversion to sustainable jet fuels, contingent on continued technological advancements and supportive economic and policy environments. Considering regional variations, leveraging policy mechanisms, and fostering international cooperation can enhance the scalability and broader applicability of the studied conversion technologies, contributing to global carbon reduction and sustainable energy goals.

While this study provides an extensive overview of the technical, economic, and environmental aspects of CO_2-CO-FTS-Fuel and CO_2-Methanol-Fuel, there is a need to explore other CO_2 utilization technologies. Future research should focus on advanced catalysis and reaction mechanisms, scalability and industrial integration, renewable hydrogen production, integration with renewable energy sources, and policy and economic incentives. By prioritizing these areas, researchers can address key barriers and enhance the feasibility and sustainability of CO_2 conversion technologies. This study contributes significantly to ongoing efforts in CO_2 reduction and renewable energy by offering a holistic techno-economic analysis, optimizing supply chain networks, conducting sensitivity analyses, assessing environmental impacts, and providing a robust framework for future research. These contributions support the development and implementation of sustainable CO_2 conversion technologies, helping to achieve global carbon reduction targets and promoting renewable energy solutions.

CRediT authorship contribution statement

Rui Zhou: Visualization, Writing – review & editing, Writing – original draft, Data curation, Resources, Investigation, Software, Methodology, Conceptualization, Formal analysis. **Mingzhou Jin:** Project administration, Supervision, Methodology, Resources, Conceptualization, Funding acquisition, Writing – review & editing. **Zhenglong Li:** Conceptualization, Investigation, Data curation, Validation, Writing – review & editing. **Yang Xiao:** Software, Writing – review & editing. **David McCollum:** Writing – review & editing. **Alicia Li:** Writing – review & editing.

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

Data is available at Github: https://github.com/rachelriri0228/TEA-and-Network-Design-for-CO2-conversion-to-Fuels-The-United-States-Case-Study.

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