Optimization-based framework for technical, economic, and environmental performance assessment of CO_2 utilization strategies

Thai Ngan Do*, Hegwon Chung*, Yunjik Lee*, Changsu Kim*, Beomsoo Kim*, Jiyong Kim*

**School of Chemical Engineering, Sungkyungkwan University, 16419, Republic of Korea*

(e-mail: jiyongkim@skku.edu).

Abstract: Carbon capture and utilization (CCU) for chemicals and fuel production is one of the effective measures addressing global warming and energy security. Since CCU utilizes harmful CO_2 as a raw material to produce high-value chemicals and fuels such as methanol, Fischer-Tropsch fuel, dimethyl ether, and gasoline, it mitigates CO_2 emission and creates more fuel availability or shares the burden on fossil fuels. This study aims to develop an optimization-based framework of CO_2 utilization strategies and to analyze CO_2-to-fuel strategies regarding technical, economic, and environmental performance. To achieve this goal, we generated a superstructure consisting of many CO_2 utilization pathways, including a series of technologies (e.g., reaction/conversion, and separation and purification) for different fuel production. We then developed process simulation and estimated the key techno-economic parameters such as mass and energy flow, and sizing and costing data. The optimization models were developed to identify the optimal CO_2 utilization strategy and assess its feasibility with four different criteria: energy efficiency (EEF), production quantity, production cost (UPC), and net CO_2 emission (NCE). As a result, the proposed optimization-based framework is able to i) identify the best CO_2 utilization strategy over various technological pathways for targeted fuels, ii) provide a decision-making guide to policymakers and stakeholders for planning an economically viable and sustainable CO_2 utilization strategy.

Keywords: CO_2 utilization superstructure; CO_2-based fuels; Process design; Techno-economic analysis, Optimization.

1. INTRODUCTION

The deployment of the carbon capture and utilization (CCU) technology framework is one of the active solutions to address environmental issues related to CO_2 emissions. While CCU covers the whole processes in a carbon lifecycle from capture, storage, transport and industrial utilization, using captured CO_2 as an alternative carbon feedstock for value-added chemical production is the most important stage. That helps mitigate CO_2 emission and ensure energy security by enlarging fuels availability/sharing burden on fossil fuels. Many CO_2 utilization technologies, such as catalytic conversion, thermochemical energizing, electrochemical reduction, have received attention, especially for methanol (MeOH), dimethyl ether (DME), Fischer-Tropsch (FT fuels) and gasoline (Kim et al., 2012; Mevawala et al., 2017). The research topics cover from catalytic/material development (Centi et al., 2013), thermodynamic and reaction kinetics, to process design, operation, optimization, techno-economic and environmental analysis (Do et al., 2022; Do & Kim, 2019, 2020). Other, a technological superstructure and optimization-based framework for fuels and chemicals from various feedstock materials has recently been spotlighted. For instances, the optimization assessment has been conducted for biomass-to-fuel strategy (Kim et al., 2013). Further, Han et al. developed the superstructure and optimization-based framework assessment for residue gas utilization (Han et al., 2019).

This study aims to develop an optimization-based framework of CO_2 utilization strategies to identify and analyze CO_2-to-fuel strategies with different evaluation criteria: energy efficiency (EEF), production quantity, production cost (UPC), and net CO_2 emission (NCE). First, the problem statement and methodology description are determined and presented (Section 2). Section 3 describes the technological superstructure generation by integrating various carbon conversion and separation technologies to produce CO_2-based fuels such as MeOH, DME, FT fuels and gasoline. Then, the process simulation of unit technology and possible CO_2-to-fuels pathways were developed for obtaining techno-economic parameters (e.g., mass and energy flow, and sizing and costing data) (Section 4). The optimization models were developed to identify the optimal CO_2-to-fuel strategies regarding maximum energy efficiency, maximum production quantity, minimum unit production cost, and minimum net CO_2 reduction, as in Section 5. Finally, the optimal CO_2 utilization strategy for targeted fuels is provided and discussed in Section 6.

2. METHODOLOGY DESCRIPTION

The goal of this study is to propose an optimization-based assessment framework for establishing CO_2 utilization strategies for targeted CO_2-based fuels. The proposed framework has four steps for establishing optimal strategies as, illustrated in Figure 1.

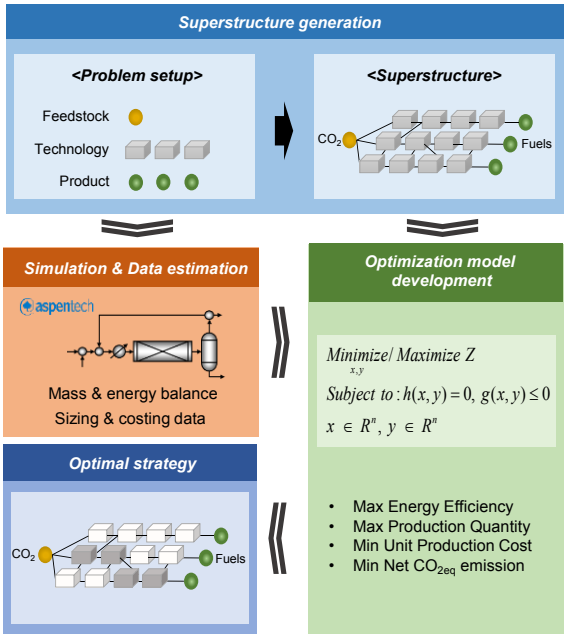


Figure 1. Methodology for the assessment of CO_2 utilization strategy for liquid fuels

- Step 1. Setup the problems by choosing captured CO_2 as a main feedstock, choosing possible technologies, and final products, and generating superstructure by integrating technologies for targeted product from CO_2.
- Step 2. Development of process simulation of every single technology and technological pathway for technical (mass and energy flows), and economic date (estimation of sizing and costing).
- Step 3. Development of optimization model for decision-making with generated data and associated parameters.
- Step 4. Identification of optimal solutions for a given problem based on a specific criterion.

3. CO_2 UTILIZATION SUPERSTRUCTURE

3.1 Compounds

In this study, the compounds used for CO_2 utilization are categorized into three groups: feedstock, intermediate, and final products. For a given initial condition of feedstock (captured CO_2), the results of intermediate and final products can be different by selecting what technologies to use. In our study of the CO_2 utilization system, the intermediates include syngas and MeOH; meanwhile, four final products are MeOH, DME, FT-fuel, and gasoline. The so-called syngas is mainly composed of H_2 and CO, which have an adjusted value of $(H_2 - CO_2)/(CO + CO_2)$. Note that MeOH belongs to the intermediate and final product at the same time. MeOH, which is used right after the purification, can be classified as a final product. On the other hand, it can also be classified as an intermediate if used for the material of synthesis of gasoline or DME.

3.2 Technologies

There are two types of technologies, conversion/reaction and separation, as listed below:

- Conversion/reaction technology: direct CO_2 hydrogenation, reverse water-gas shift, thermochemical CO_2 energizing, electrochemical CO_2 reduction, methanol/DME/FT synthesis, methanol-to-gasoline, methanol dehydration.
- Separation technology: CO_2 absorption, CO adsorption, flash-tank, and distillation.

3.3 Superstructure for CO_2 utilization

The superstructure in the study is composed of two types of technologies and three types of compounds. Then, we can construct 43 pathways for CO_2 utilization, as shown in Figure 2. CO_2 can be converted into four different products which can be used as a liquid fuel through multiple strategies. For example, FT-fuel can be produced directly from the feedstock using direct hydrogenation or through the Fischer-Tropsch synthesis process from syngas intermediate. The superstructure for liquid fuel generation from CO_2 can be extended by adding other strategies which have different combinations of conversion and separation technologies. Note that a single technology includes various operating equipment.

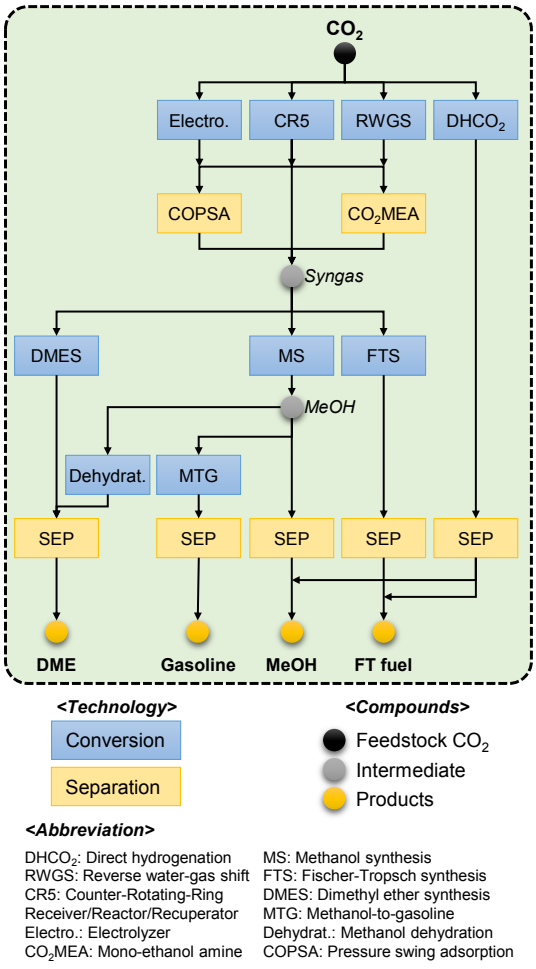


Figure 2. Superstructure of CO_2 utilization to fuels

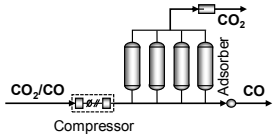
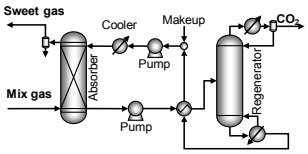
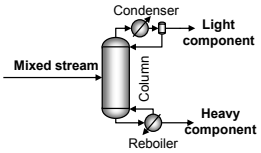
4. SIMULATION AND PARAMETER ESTIMATION

Using the information of the generated superstructure, we developed process model of involved technologies and possible pathways using Aspen Plus V.11. The major assumptions and description of single conversion and separation technologies were summarized in Table 1 and Table 2, respectively.

Table 1. Major assumptions and description of conversion technologies (Do et al., 2022)

Technology	Operating condition	Description
Reverse water gas shift (RWGS)	400-1,200°C 1-20 bar	This is reverse reaction of water gas shift, produces CO and H_2O from CO_2 and H_2 $CO_2 + H_2 \leftrightarrow CO + H_2O$
Direct CO_2 hydrogenation (DHCO2) to MeOH	250-350 °C 35-55 bar	Under catalyst activation, CO_2 is directly hydrogenated to CO and subsequently converted to methanol using Cu/Zn/Al/Zr catalyst. $CO_2 + H_2 \leftrightarrow CO + H_2O$ $CO_2 + 3H_2 \rightarrow CH_3OH$ $CO + 2H_2 \rightarrow CH_3OH$
Direct CO_2 hydrogenation (DHCO2) to FT fuels	300 °C 25 bar	Fe-based catalyst is used in two-stage conversion of direct hydrogenation: CO_2 hydrogenated to CO, and FT syntheis.
Counter-Rotating-Ring Receiver/Reactor/ Recuperator (CR5)	~1500 °C	Chemical bond of CO_2 and H_2O is broken, forming CO and H_2 under high-temperature flux of concentarted solar energy and reactive material contained in CR5.
Electrolyzer for CO2 reduction (Elecz.)	1-30 bar	The key component CO_2 electrolyzer. Its contains electrocatalyst for CO_2 reduction and H_2O oxidation. It requires electrical energy for operation.
Methanol synthesis (MS)	150-300 °C 50-75 bar	The commercial technology used the catalyst of Cu/ZnO/Al_2O_3 to produce methanol from syngas $CO + H_2 \rightarrow CH_3OH$
Dimethyl ether synthesis (DMES)	200-400 °C 20-60 bar	Bifunctional catalyst of CuO/ZnO/Al_2O_3 and γ-Al_2O_3 is used to synthesize DME from syngas, including reactions: $CO + H_2 \rightarrow CH_3OH$ $2CH_3OH \rightarrow CH_3OCH_3 + H_2O$
Fischer-Tropsch synthesis (FTS)	200-250 °C 25-60 bar	FT fuel is synthesized from syngas. $nCO + 2nH_2 \rightarrow -(CH_2)_n - + nH_2O$
Methanol-to-gasoline (MTG)	300-400 °C 10-20 bar	The industrial process converts methanol to hydrocarbon using HSZM-5. $CH_3OH \rightarrow -(CH_2) - + nH_2O$
Dehydration of methanol to DME (Dehydr)	250-400 °C 2-20 bar	Dehydration of methanol to DME takes place on a γ-Al_2O_3, as reaction: $2CH_3OH \rightarrow CH_3OCH_3 + H_2O$

Table 2. Simplified process flow diagram of separation technologies

Technology	Description	Process flow diagram
CO Pressure Swing Adsorption (CO-PSA)	Component separation of CO	
CO_2 mono-ethanolamine Absorption (CO2MEA)	Component separation of CO_2	
Distillation	Separation of all liquid streams	

By connecting various technologies, many possible CO_2-to-fuels pathways was developed. With the rigorous models, the mass flow, energy flow, sizing and costing data were then obtained for the optimization model's input and further analysis, which is presented in Table 3.

5. OPTIMIZATION MODEL

To identify the optimal CO_2 utilization strategies, we develop an optimization model using a mixed-integer linear programming (MILP) technique.

5.1 Objective function

This work considers various criteria as an objective function to determine the best CO_2 utilization strategy for each fuel. Therein, we developed optimization for four different objective functions regarding energy efficiency, production quantity, production cost, and net CO_2 emission.

Maximum energy efficiency: (1) is used to identify the optimal strategy with the maximum energy efficiency, which means maximum energy captured and stored in targeted fuels (for a certain input of energy/utility).

$$max\ Z_1 = \sum_j (1 - f_i - u_i) \quad (1)$$

where f_i is the heating value of feedstock $i \epsilon I^F$, and u_i is the energy consumption of utility $i \epsilon I^U$ required for one energy unit of product.

Maximum production quantity: with a given amount of feedstock, the amount of targeted product can be different through different technological pathways. The objective function (2) is used to identify the strategy with the maximum amount of targeted product (from a given amount of feedstock).

Table 3. Major techno-economic and environmental data

No.	Technological pathway		Input (ton/h)	Output (ton/h)	Yield	TCI (M$)	TOC (M$/y)	ER (MW)	DCE ($tonCO_2$/h)
1	RWGS-MS-SEP	MeOH_1	437.9	249.9	0.57	664	2,093	759	36.7
2	CR5-MS-SEP	MeOH_2	433.3	253.5	0.59	10,934	1,875	679	32.8
3	ELECZ-MS-SEP	MeOH_3	431.7	255.5	0.59	3,243	1,900	990	30.4
4	RWGS-COPSA-MS-SEP	MeOH_4	439.1	259.4	0.59	3,639	2,462	708	26.5
5	CR5-COPSA-MS-SEP	MeOH_5	425.3	256.5	0.60	35,241	2,156	567	29.2
6	ELECZ-COPSA-MS-SEP	MeOH_6	426.2	264.3	0.62	7,291	2,091	1,169	18.8
7	RWGS-CO2MEA-MS-SEP	MeOH_7	437.2	253.1	0.58	692	2,204	1,699	33.8
8	CR5-CO2MEA-MS-SEP	MeOH_8	424.2	256.6	0.60	31,874	1,677	1,322	29.2
9	ELECZ-CO2MEA-MS-SEP	MeOH_9	425.6	263.9	0.62	5,430	1,953	1,873	18.9
10	DHCO2MEOH-SEP	MeOH_10	440.1	270.4	0.61	734	2,068	383	14.6
11	RWGS-COPSA-FTS-SEP	FT_fuel_1	443.5	82.3	0.19	4,048	2,805	1,217	6.3
12	CR5-COPSA-FTS-SEP	FT_fuel_2	429.5	81.7	0.19	35,644	2,486	1,032	7.5
13	ELECZ-COPSA-FTS-SEP	FT_fuel_3	429.6	83.6	0.19	7,701	2,399	1,691	4.5
14	RWGS-CO2MEA-FTS-SEP	FT_fuel_4	442.2	79.9	0.18	1,016	2,561	2,146	9.8
15	CR5-CO2MEA-FTS-SEP	FT_fuel_5	428.4	81.7	0.19	32,229	2,000	1,776	7.5
16	ELECZ-CO2MEA-FTS-SEP	FT_fuel_6	429.0	83.6	0.19	5,798	2,248	2,364	4.5
17	DHCO2FT-SEP	FT_fuel_7	442.8	119.2	0.27	880	2,203	438	145.9
18	RWGS-MS-DEHYDR-SEP	DME_1	437.9	179.5	0.41	1,250	2,149	992	36.7
19	CR5-MS-DEHYDR-SEP	DME_2	433.3	182.1	0.42	11,526	1,932	915	32.8
20	ELECZ-MS-DEHYDR-SEP	DME_3	431.7	183.6	0.43	3,837	1,957	1,228	30.4
21	RWGS-COPSA-MS-DEHYDR-SEP	DME_4	439.1	186.4	0.43	4,240	2,520	949	26.5
22	CR5-COPSA-MS-DEHYDR-SEP	DME_5	425.3	184.3	0.43	35,837	2,213	805	29.2
23	ELECZ-COPSA-MS-DEHYDR-SEP	DME_6	426.2	189.8	0.45	7,899	2,151	1,415	18.8
24	RWGS-CO2MEA-MS-DEHYDR-SEP	DME_7	437.2	181.9	0.42	1,283	2,261	1,935	33.8
25	CR5-CO2MEA-MS-DEHYDR-SEP	DME_8	424.2	184.3	0.43	32,470	1,734	1,561	29.2
26	ELECZ-CO2MEA-MS-DEHYDR-SEP	DME_9	425.6	189.6	0.45	6,038	2,012	2,118	18.9
27	DHCO2MEOH-DEHYDR-SEP	DME_10	440.1	194.3	0.44	1,351	2,129	635	14.6
28	RWGS-COPSA-DMES-SEP	DME_11	417.6	179.5	0.43	3,573	1,679	511	182.2
29	CR5-COPSA-DMES-SEP	DME_12	402.2	95.6	0.24	35,170	1,307	315	183.7
30	ELECZ-COPSA-DMES-SEP	DME_13	407.0	113.8	0.28	7,250	1,405	1,041	159.1
31	RWGS-CO2MEA-DMES-SEP	DME_14	410.4	80.5	0.20	434	1,200	1,355	215.9
32	CR5-CO2MEA-DMES-SEP	DME_15	401.1	95.7	0.24	31,770	813	1,049	195.7
33	ELECZ-CO2MEA-DMES-SEP	DME_16	406.3	113.9	0.28	5,348	1,253	1,713	159.1
34	RWGS-MS-MTG	Gasoline_1	437.9	140.6	0.27	1,520	2,054	527	11.4
35	CR5-MS-MTG	Gasoline_2	433.3	147.4	0.29	11,814	1,834	435	6.4
36	ELECZ-MS-MTG	Gasoline_3	431.7	133.2	0.26	4,064	1,863	769	4.7
37	RWGS-COPSA-MS-MTG	Gasoline_4	438.1	114.2	0.22	4,381	2,045	537	5.4
38	CR5-COPSA-MS-MTG	Gasoline_5	424.1	116.7	0.23	35,993	1,673	363	6.7
39	ELECZ-COPSA-MS-MTG	Gasoline_6	425.6	110.0	0.22	8,016	1,819	1,019	2.9
40	RWGS-CO2MEA-MS-MTG	Gasoline_7	437.2	122.7	0.24	1,453	2,165	1,464	9.7
41	CR5-CO2MEA-MS-MTG	Gasoline_8	424.2	116.8	0.24	32,627	1,642	1,119	6.7
42	ELECZ-CO2MEA-MS-MTG	Gasoline_9	425.6	110.1	0.22	6,157	1,933	1,754	2.9
43	DHCO2MEOH-MTG	Gasoline_10	440.1	163.9	0.32	1,701	2,034	176	6.0

[a] Yield: calculated based on the material input and production output.
[b] TCI (M$): total capital investment cost.
[c] TOC (M$/y): total annual operating cost
[d] ER (MWh): energy requirement for process.
[e] DCE (ton/h): direct CO_{2eq} emission (vent-out gas, purge gas) from process.
Abbreviations: RWGS: Reverse water-gas shift, DH: Direct CO_2 hydrogenation, CR5: Counter-Rotating-Ring Receiver/Reactor/ Recuperator, ELECZ: Electrochemical reduction, MS: Methanol synthesis, FTS: Fischer–Tropsch synthesis, DMES: dimethylether synthesis, DEHYDR.: Methanol dehydration, MTG: methanol-to-gasoline, COPSA: CO separation by adsorption, CO2MEA: CO2 separation by absorption, SEP: separation and purification.

$$max\ Z_2 = \sum_j P_i \qquad (2)$$

Minimum unit production cost: the objective function (3) seeks for the strategy with minimum unit production cost for a certain amount of targeted product.

$$min\ Z_3 = \sum_j \alpha_j + \sum_j \psi_j + \sum_{i \epsilon I^F} \xi_i F_i + \sum_{i \epsilon I^U} \omega_i U_{ij} \qquad (3)$$

where α_j and ψ_j is the annualized capital cost and fixed operating cost of technological pathway j; ξ_i and ω_i the unit price of feedstock $i \epsilon I^F$ and utility $i \epsilon I^U$ in technological pathway j.

Minimum net CO_2 emission: if the goal is to find the most eco-friendly strategy to a certain amount of target product, then we use (4) to identify the minimum net CO_2 emission strategy. It

includes direct CO_2 emission of pathway, indirect CO_2 emission via utility consumption, and feedstock inventory.

$$min\ Z_4 = \sum_j \lambda_j + \sum_{i \epsilon I^U} \varepsilon_i U_{ij} - \sum_{i \epsilon I^F} \tau_i F_i \qquad (4)$$

where λ_j is the direct emission from technological pathway j; ε_i is CO_2 equivalent factor of unit utility $i \epsilon I^U$ consumed in technological pathway j, τ_i is the CO_2 equivalent factor of feedstock $i \epsilon I^F$ in technological pathway j.

5.2 Constraints

Feedstock availability and minimum purchase: the feedstock purchase is upper bounded of minimum purchase and lower bounded by feed's availability as in (5):

$$\gamma_i \leq F_i \leq \delta_i \qquad (5)$$

Demand satisfaction: The optimization model was constrained by demands for final product β_i as expressed in (6):

$$P_i \geq \beta_i \qquad (6)$$

6. RESULTS AND DISCUSSION

6.1 Optimal strategy for methanol

Figure 3 presents the optimal strategy for MeOH with different criteria. The optimal CO_2-to-MeOH strategy regarding maximum EEF is through pathways of thermochemical CO_2 energizing followed by methanol synthesis at 82.7%. However, its UPC is around 5-time higher than others. The most economic and eco-friendly strategy is the direct CO_2 hydrogenation with the production rate of 270.4 ton/h, UPC at 0.68 \$/kg and NCE at -0.19 $kgCO_2/kg$ (reduces CO_{2eq} emission with negative NCE).

6.2 Optimal strategy for dimethyl ether

The optimal strategies for DME production are presented in Figure 4. The thermochemical splitting (CR5) subsequent DME synthesis is the optimal CO_2-to-DME strategy for maximum EEF at 93.9%, but extremely high UPC. Meanwhile, the strategy with direct hydrogenation to methanol – dehydration to DME is the best for techno-economic and environmental performance, which results in 194.3 ton/h, 1.05\$/kg and 0.05 $kgCO_2/kg$.

6.3 Optimal strategy for Fischer-Tropsch fuel

Figure 5 summarizes the optimal CO_2-to-FT fuel strategies and its key indicator. The direct CO_2 hydrogenation to FT fuels is outstanding strategy, which is the optimal one for all four examined criteria. FT fuels is product with production rate at 119.2 ton/h, EEF at 58.2%, UPC at 1.67 \$/kg, and NCE at 1.21 $kgCO_2/kg$.

6.4 Optimal strategy for gasoline

For gasoline production, the optimal strategies and its description are presented in Figure 6. The direct hydrogenation to methanol subsequent methanol-to-gasoline is the optimal strategy for maximum EEF at 81.3%, maximum product quantity at 140 ton/h, and minimum UPC at 1.42 \$/kg. It is also an eco-friendly strategy (reduce 0.71 $kgCO_2/kg$). The best environmental strategy is thermochemical energizing subsequent methanol synthesis and methanol-to-gasoline, which reduce 1.06 $kgCO_2/kg$ gasoline. However, this strategy is worst in techno-economic performance at low efficiency and high production cost.

Problem	Optimal Strategy (CO_2-to-methanol)	Optimal value	Other criteria
(a) Max EEF	CO_2 → CR5 → COPSA → MS → SEP → MeOH	82.7%	• Amount: 256.5 ton/h • UPC: 3.44 \$/kg • NCE: -0.18 $kgCO_2/kg$
(b) Max Amount	CO_2 → $DHCO_2$ → SEP → MeOH	270.4 ton/h	• EEF: 71.2% • UPC: 0.68 \$/kg • NCE: -0.19 $kgCO_2/kg$
(c) Min UPC	CO_2 → $DHCO_2$ → SEP → MeOH	0.68 \$/kg	• EEF: 71.2% • Amount: 270.4 ton/h • NCE: -0.19 $kgCO_2/kg$
(d) Min NCE	CO_2 → $DHCO_2$ → SEP → MeOH	-0.19 $kgCO_2/kg$	• EEF: 71.2% • Amount: 270.4 ton/h • UPC: 0.68 \$/kg

Figure 3. Optimal strategy for methanol production using different criteria

Problem	Optimal Strategy (CO_2-to-DME)	Optimal value	Other criteria
(a) Max EEF	CO_2 → CR5 → COPSA → DMES → SEP → DME	93.9%	• Amount: 95.6 ton/h • UPC: 8.51 \$/kg • NCE: 0.64 $kgCO_2/kg$
(b) Max Amount	CO_2 → $DHCO_2$ → Dehydrat. → SEP → DME	194.3 ton/h	• EEF: 58.4% • UPC: 1.05 \$/kg • NCE: 0.05 $kgCO_2/kg$
(c) Min UPC	CO_2 → $DHCO_2$ → Dehydrat. → SEP → DME	1.05 \$/kg	• EEF: 58.4% • Amount: 194.3 ton/h • NCE: 0.05 $kgCO_2/kg$
(d) Min NCE	CO_2 → $DHCO_2$ → Dehydrat. → SEP → DME	0.05 $kgCO_2/kg$	• EEF: 58.4% • Amount: 194.3 ton/h • UPC: 0.68 \$/kg

Figure 4. Optimal strategy for DME production using different criteria

Problem	Optimal Strategy (CO_2-to-FT fuel)	Optimal value	Other criteria
(a) Max EEF	CO_2 → $DHCO_2$ → SEP → FT fuel	58.2%	• Amount: 119.2 ton/h • UPC: 1.67 $/kg • NCE: 1.21 $kgCO_2/kg$
(b) Max Amount	CO_2 → $DHCO_2$ → SEP → FT fuel	119.2 ton/h	• EEF: 58.2% • UPC: 1.67 $/kg • NCE: 1.21 $kgCO_2/kg$
(c) Min UPC	CO_2 → $DHCO_2$ → SEP → FT fuel	1.67 $/kg	• EEF: 58.2% • Amount: 119.2 ton/h • NCE: 1.21 $kgCO_2/kg$
(d) Min NCE	CO_2 → $DHCO_2$ → SEP → FT fuel	1.21 $kgCO_2/kg$	• EEF: 58.2% • Amount: 119.2 ton/h • UPC: 1.67 $/kg

Figure 5. Optimal strategy for FT fuel production using different criteria

Problem	Optimal Strategy (CO_2-to-gasoline)	Optimal value	Other criteria
(a) Max EEF	CO_2 → $DHCO_2$ → MTG → SEP → Gasoline	81.3%	• Amount: 140.0 ton/h • UPC: 1.42 $/kg • NCE: -0.71 $kgCO_2/kg$
(b) Max Amount	CO_2 → $DHCO_2$ → MTG → SEP → Gasoline	140.0 ton/h	• EEF: 81.3% • UPC: 1.42 $/kg • NCE: -0.71 $kgCO_2/kg$
(c) Min UPC	CO_2 → $DHCO_2$ → MTG → SEP → Gasoline	1.42 $/kg	• EEF: 81.3% • Amount: 140.0 ton/h • NCE: -0.71 $kgCO_2/kg$
(d) Min NCE	CO_2 → CR5 → SEP → MS → MTG → Gasoline	-1.06 $kgCO_2/kg$	• EEF: 72.3% • Amount: 99.7 ton/h • UPC: 8.39 $/kg

Figure 6. Optimal strategy for gasoline production using different criteria

7. CONCLUSION

This study developed an optimization-based assessment framework for CO_2-to-fuel strategies, based on the CO_2 utilization superstructure, which includes a number of conversion and separation technologies for desired fuel production. The optimization-based assessment framework enables us to identify CO_2 utilization strategies for different fuel production regarding various evaluated criteria: maximum energy efficiency, maximum production quantity, minimum unit production cost, and minimum net CO_2 emission. The framework supports policymakers and stakeholders in identifying suitable strategic solutions in utilizing CO_2 for different targeted fuels with different criteria.

REFERENCES

Centi, G., Quadrelli, E. A., & Perathoner, S. (2013). Catalysis for CO2 conversion: A key technology for rapid introduction of renewable energy in the value chain of chemical industries. In *Energy and Environmental Science* (Vol. 6, Issue 6, pp. 1711–1731). https://doi.org/10.1039/c3ee00056g

Do, T. N., & Kim, J. (2019). Process development and techno-economic evaluation of methanol production by direct CO2 hydrogenation using solar-thermal energy. *Journal of CO2 Utilization*, *33*, 461–472. https://doi.org/10.1016/j.jcou.2019.07.003

Do, T. N., & Kim, J. (2020). Green C2-C4 hydrocarbon production through direct CO2 hydrogenation with renewable hydrogen: Process development and techno-economic analysis. *Energy Conversion and Management*, *214*, 112866. https://doi.org/10.1016/j.enconman.2020.112866

Do, T. N., You, C., & Kim, J. (2022). A CO 2 utilization framework for liquid fuels and chemical production: techno-economic and environmental analysis. *Energy & Environmental Science*, *15*(1), 169–184. https://doi.org/10.1039/d1ee01444g

Han, S., Kim, S., Kim, Y. T., Kwak, G., & Kim, J. (2019). Optimization-based assessment framework for carbon utilization strategies: Energy production from coke oven gas. *Energy Conversion and Management*, *187*, 1–14. https://doi.org/10.1016/j.enconman.2019.03.007

Kim, J., Johnson, T. A., Miller, J. E., Stechel, E. B., & Maravelias, C. T. (2012). Fuel production from CO 2 using solar-thermal energy: System level analysis. *Energy and Environmental Science*, *5*(9), 8417–8429. https://doi.org/10.1039/c2ee21798h

Kim, J., Sen, S. M., & Maravelias, C. T. (2013). An optimization-based assessment framework for biomass-to-fuel conversion strategies. *Energy and Environmental Science*, *6*(4), 1093–1104. https://doi.org/10.1039/c3ee24243a

Mevawala, C., Jiang, Y., & Bhattacharyya, D. (2017). Plant-wide modeling and analysis of the shale gas to dimethyl ether (DME) process via direct and indirect synthesis routes. *Applied Energy*, *204*, 163–180. https://doi.org/10.1016/j.apenergy.2017.06.085