

**Electronic Supplementary Information:**

**CO<sub>2</sub> utilization framework for liquid fuels and chemicals: Techno-economic  
and environmental analysis**

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## S1. Potential of CO<sub>2</sub> utilization for energy-based product (CCU4E)

**Table S1.1.** The current and potential of supply and demand of CO<sub>2</sub>

	Supply	Mtpa	Demand*	Mtpa
Current	Natural geological CO <sub>2</sub> reservoirs	55	EOR	80
	Industrial by-products	55	Food industry	7
			Beverage carbonation	7
			Fabrication of metal	5
			Other applications	10
Future	Current supply (2019)	110	Growth of existing demand	200
	Growth of existing supply to (2030)	90	EGS	5 – 30
	Bulk CO <sub>2</sub> (low cost)	500	ECBM	30 – 300
	Bulk CO <sub>2</sub> (medium cost)	2,000	EOR & EGR	30 – 300
	Bulk CO <sub>2</sub> (high cost)	18,000	Polymer processing	5 – 30
			Bauxite treatment	5 – 30
			Carbonate aggregates	30 – 300
			CO <sub>2</sub> cement curing	60 – 600
		Surplus to energy-based product	>910	

\* The estimation do not consider the use of CO<sub>2</sub> in the urea manufacturing <sup>1</sup>.

The potential supply and future demand for CO<sub>2</sub> production are not readily available, which is provided of the order of magnitude, as reviewed by Global CCS Institute [1] and where else <sup>2,3</sup>. The global consumption of CO<sub>2</sub> is currently estimated to be 110 Mtpa (2020) in which the large volume of CO<sub>2</sub> onsite-generated and directly consumed in urea manufacturing is excluded <sup>2</sup>. About 80 Mtpa CO<sub>2</sub> is consumed for enhanced oil recovery (EOR) whereas the remain is supplied for the food and beverage industry, fabrication of metal, and others.

Since a small portion of CO<sub>2</sub> has been industrially utilized, the huge potential emission sources at the different concentrated levels corresponded to the CO<sub>2</sub> captured cost was reported by IPCC <sup>4</sup>. The potential supply of CO<sub>2</sub> from large point sources is estimated at 500 Mtpa of low-cost of high-concentrated CO<sub>2</sub>, 2,000 Mtpa of medium cost, and 18,000 Mtpa of high-cost of CO<sub>2</sub> <sup>1</sup>. With the consideration of using only the low- and medium-cost of captured CO<sub>2</sub>, there is still very large unbalance between CO<sub>2</sub> demand and supply. The current use of CO<sub>2</sub> is estimated to 2030 at roughly 200 Mtpa <sup>2</sup>. Several existed and emerging technology have been considered for the large potential use of CO<sub>2</sub> as sequestered underground or utilized for materials, chemicals, and fuels. Eventually, the high scenarios of the use of CO<sub>2</sub> for sequestration and CO<sub>2</sub>-based materials were estimated, there is still a large surplus of CO<sub>2</sub> for chemical and fuel that have vast demand. That has driven effort to develop technology of CO<sub>2</sub> utilization into chemical and fuel production that have vast demand. The potential fuel production of CO<sub>2</sub> utilization was reviewed and estimated based on the current market size considered the annual growth rate to 2030 <sup>5</sup>.

While a number of fuels and chemicals can be produced through different technological combinations, we selected eight different products and representative 72 pathways based on several considerations such as commercialization, fully accessible information, technology maturity, especially potential market size of these products in future. The potential market size of CO<sub>2</sub>-based fuels was estimated followed the methodology of Reference <sup>5</sup>, and presented in Table S1.2.

**Table S1.2.** The potential market size of liquid fuels from CO<sub>2</sub> utilization

Product	Potential production of CO <sub>2</sub> utilization in 2030 (Mt/y)
Methanol	204 <sup>a</sup>
Ethanol	163 <sup>b</sup>
Olefin	7 <sup>c</sup>
Gasoline	2154 <sup>d</sup> (to Infinite)
Fischer-Tropsch fuel	163 <sup>e</sup>
Bio-diesel	176 <sup>f</sup>
Dimethyl ether	41 <sup>e</sup>
Formic acid	10 <sup>g</sup>

<sup>a</sup> Estimated in high scenario for methanol as a chemical feedstock and fuel, based on Ref <sup>5</sup>

<sup>b</sup> The annual growth of ethanol is assumed at 6%, and 85% of market share in 2030 <sup>5,6</sup>

<sup>c</sup> Estimated in high scenario for olefin (mainly ethylene and propylene), based on Ref <sup>5</sup>

<sup>d</sup> Estimated based on global oil demand (105.4 million barrel per day in 2030) <sup>7</sup>

<sup>e</sup> Estimated in high scenario based on Ref [7]

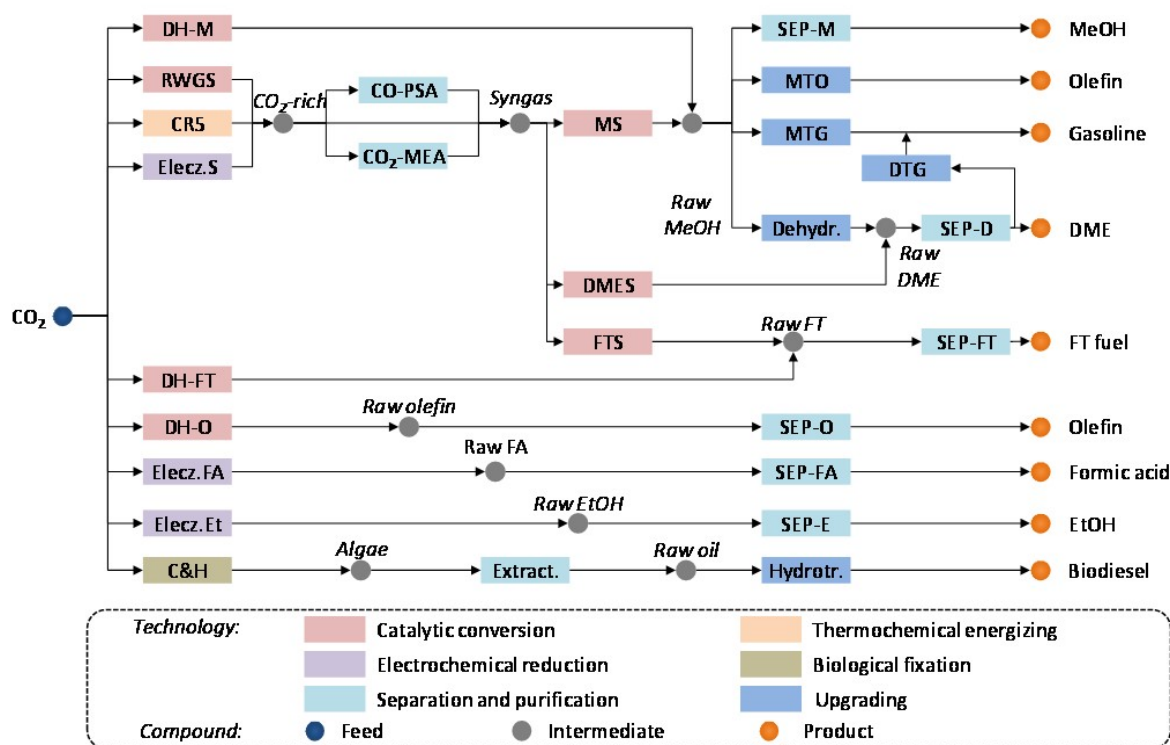
<sup>f</sup> Estimated from 115 Mt in 2018 with the growth of 3.6% per year <sup>8</sup>

<sup>g</sup> Taken from Ref <sup>9</sup>

## S2. Process simulation and modeling

### S2.1. Simulation of each technology

Based on the generated superstructure, summarized in Fig. S2.1, the unit technologies were firstly simulated using Aspen Plus software, subsequent full CO<sub>2</sub>-to-fuel pathways. Here, each technology consists of various equipment for its operation purpose (e.g., reaction kinetic expressions, temperature, pressure, etc.) that was detailed described in Table S2.1.

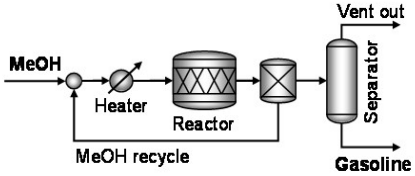
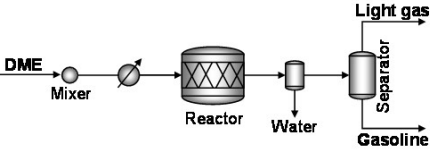
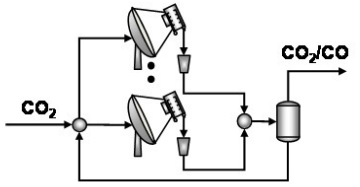
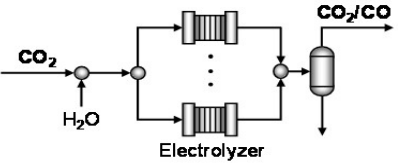
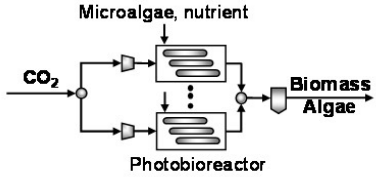


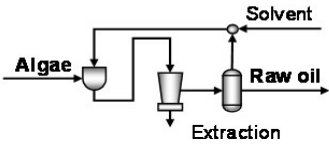
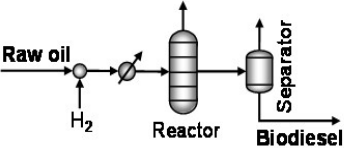
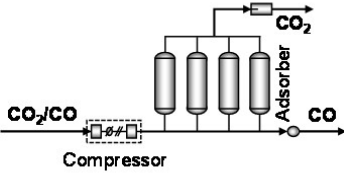
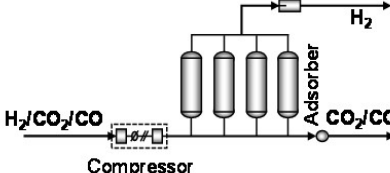
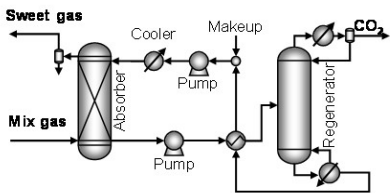
**Fig. S2.1.** The CCU4E superstructure. Abbreviation: RWGS: Reverse water-gas shift, DH-M: Direct hydrogenation to methanol, DH-FT: Direct hydrogenation to Fischer-Tropsch, DH-O: Direct hydrogenation to olefin, CR5: Counter-Rotating-Ring/Receiver/Reactor/Recuperator, Elec.z.S: Electrochemical reduction to syngas, Elec.z.FA: Electrochemical reduction to formic acid, Elec.z.EtOH: Electrochemical reduction to ethanol, MS: Methanol synthesis, FTS: Fischer-Tropsch synthesis, DMES: Dimethyl ether synthesis, C&H: cultivation and harvesting, Extract.: Oil extraction, Hydrotr.: Hydrotreating, Dehydro.: Dehydration, MTO: methanol-to-olefin, MTG: Methanol-to-gasoline, DTG: dimethyl ether-to-gasoline, CO-PSA: CO Pressure Swing Adsorption, CO<sub>2</sub>-MEA: CO<sub>2</sub> Absorption by monoethanolamine, SEP-M, SEP-D, SEP-FT, SEP-O, SEP FA, SEP-E: Separation and purification for methanol, dimethyl ether, FT fuel, olefin, formic acid, ethanol.

**Table S2.1.** Unit process specification and parameters for simulation

Process	Simplified PFD	Operating conditions		
		T (°C)	P (bar)	Description
Reverse water gas shift (RWGS)		400-1,200	1-20	$r_1 = \frac{k_2 P_{CO_2} (1 - P_{H_2O} P_{CO} / k_{e,2} P_{H_2} P_{CO_2})}{(1 + K_1 P_{H_2}^{0.5} + K_2 P_{H_2O} + K_3 P_{H_2O} / P_{H_2})} \quad 10,11$
Methanol synthesis (MS)		150-300	50-75	$r_2 = \frac{k_2 P_{CO_2} (1 - P_{H_2O} P_{CO} / k_{e,2} P_{H_2} P_{CO_2})}{(1 + K_1 P_{H_2}^{0.5} + K_2 P_{H_2O} + K_3 P_{H_2O} / P_{H_2})}, r_3 = \frac{k_1 P_{CO_2} P_{H_2} (1 - P_{H_2O} P_{MeOH} / k_{e,1} P_{H_2}^3 P_{CO_2})}{(1 + K_1 P_{H_2}^{0.5} + K_2 P_{H_2O} + K_3 P_{H_2O} / P_{H_2})^3} \quad 10$
Fischer-Tropsch synthesis (FTS)		200-250	25-60	$r_1 = \frac{ae^{-b/RT} K_7^{0.5} P_{H_2}^d}{(1 + K_7^{0.5} (2 + 1 / K_4) P_{H_2}^{0.5} + \frac{K_7^{0.5}}{K_3 P_4 P_{H_2}^{-0.5}} + \frac{K_7^{0.5} P_{H_2O}}{K_2 K_3 K_4 P_{H_2}^{1.5}})} \quad 12$
Dimethyl ether synthesis (DMES)		200-400	20-60	$r_1 = \frac{k_1 f_{CO} f_{H_2}^2 [1 - f_{MeOH} / (K_1 f_{CO} f_{H_2}^2)]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2} + K_{H_2} f_{H_2})^3}, r_2 = \frac{k_2 f_{CO_2} f_{H_2}^3 [1 - f_{MeOH} f_{H_2O} / (K_2 f_{CO_2} f_{H_2}^3)]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2} + K_{H_2} f_{H_2})^4}$ $r_3 = \frac{k_3 f_{H_2O} [1 - f_{CO_2} f_{H_2} / (K_3 f_{CO} f_{H_2O})]}{1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2} + \sqrt{K_{H_2} f_{H_2}}}, r_4 = \frac{k_4 f_{MeOH} [1 - f_{DME} f_{H_2O} / (K_4 f_{MeOH}^2)]}{(1 + \sqrt{K_{MeOH} f_{MeOH}})^2}, \quad 13,14$

Direct CO <sub>2</sub> hydrogenation to methanol (DH-M)		250-350	35-55	$r_1 = k_1 \left( K_{CO} f_{CO} f_{H_2}^{1.5} - \frac{K_{CO}}{K_A} f_{CH_3OH} f_{H_2}^{-0.5} \right) / ABS,$ $r_2 = k_2 \left( K_{CO_2} f_{CO_2} f_{H_2} - \frac{K_{CO_2}}{K_B} f_{H_2O} f_{CO} \right) / ABS,$ $r_3 = k_3 \left( K_{CO_2} f_{CO_2} f_{H_2}^{1.5} - \frac{K_{CO_2}}{K_C} f_{H_2O} f_{CH_3OH} f_{H_2}^{-1.5} \right) / ABS,$ $ABS = f_{H_2}^{0.5} + \frac{K_{H_2O}}{K_H^{0.5}} f_{H_2O} + K_{CO} f_{CO} f_{H_2}^{0.5} + \frac{K_{CO} K_{H_2O}}{K_H^{0.5}} f_{CO} f_{H_2O} + K_{CO_2} f_{CO_2} f_{H_2}^{0.5} + \frac{K_{CO_2} K_{H_2O}}{K_H^{0.5}} f_{CO_2} f_{H_2O}$
Direct CO <sub>2</sub> hydrogenation to FT fuel (DH-FT)		300	25	<p>The FT synthesis considered hydrogenation of both CO<sub>2</sub> and CO, followed by reference <sup>16</sup>:</p> $nCO_2 + 3nH_2 \rightarrow -(CH_2)_n + 2nH_2O,$ $nCO + 2nH_2 \rightarrow -(CH_2)_n + nH_2O$
Direct CO <sub>2</sub> hydrogenation to olefin (DH-O)		290-360	10	$r_1 = k_1 \frac{P_{CO_2} P_{H_2} - P_{CO} P_{H_2O} / K_{eq}}{P_{CO} + a_1 P_{H_2O} + b_1 P_{CO_2}}, \quad r_i = k_i \frac{P_{CO} P_{H_2}}{P_{CO} + a_i P_{H_2O} + b_i P_{CO_2}},$
Dehydration of methanol to DME (Dehydr)		250-400	2-20	$r = \frac{k_s K_{MeOH}^2 (C_{MeOH}^2 + C_{water} C_{DME} / K_{eq})}{(1 + 2\sqrt{K_{MeOH} C_{MeOH}} + K_{water} C_{water})^4},$
Methanol-to-olefin (MTO)		490	2.2	<p>The black box model was adopted for the reactor. Mass balance and energy balance was followed by reference <sup>19</sup>.</p> $nCH_3OH \rightarrow C_n H_{2n} + nH_2O, \quad n = 2, 3, 4$

Methanol-to-gasoline (MTG)		300-400	10-20	<p>The black box model was adopted for the reactor.</p> <p>Mass balance and energy balance was followed by reference <sup>20,21</sup></p> $\frac{n}{2} [2\text{CH}_3\text{OH} \Leftrightarrow \text{CH}_3\text{OCH}_3 + \text{H}_2\text{O}] \rightarrow \text{C}_n\text{H}_{2n} + n\text{H}_2\text{O} \rightarrow n[\text{C}_n\text{H}_{2n}] + n\text{H}_2\text{O}$
Dimethyl ether-to gasoline (DTG)		200-400	20-60	$r_1 = \frac{k_1 f_{\text{CO}} f_{\text{H}_2}^2 [1 - f_{\text{MeOH}} / (K_1 f_{\text{CO}} f_{\text{H}_2}^2)]}{(1 + K_{\text{CO}} f_{\text{CO}} + K_{\text{CO}_2} f_{\text{CO}_2} + K_{\text{H}_2} f_{\text{H}_2})^3}, r_2 = \frac{k_2 f_{\text{CO}_2} f_{\text{H}_2}^3 [1 - f_{\text{MeOH}} f_{\text{H}_2\text{O}} / (K_2 f_{\text{CO}_2} f_{\text{H}_2}^3)]}{(1 + K_{\text{CO}} f_{\text{CO}} + K_{\text{CO}_2} f_{\text{CO}_2} + K_{\text{H}_2} f_{\text{H}_2})^4},$ $r_3 = \frac{k_3 f_{\text{H}_2\text{O}} [1 - f_{\text{CO}_2} f_{\text{H}_2} / (K_3 f_{\text{CO}} f_{\text{H}_2\text{O}})]}{1 + K_{\text{CO}} f_{\text{CO}} + K_{\text{CO}_2} f_{\text{CO}_2} + \sqrt{K_{\text{H}_2} f_{\text{H}_2}}}, r_4 = \frac{k_4 f_{\text{MeOH}} [1 - f_{\text{DME}} f_{\text{H}_2\text{O}} / (K_4 f_{\text{MeOH}}^2)]}{(1 + \sqrt{K_{\text{MeOH}} f_{\text{MeOH}}})^2}, \quad 22-24$
Counter-Rotating-Ring Receiver/Reactor/Recuperator (CR5)		~1500	-	<p>Collecting solar energy and converting CO<sub>2</sub> into CO. <sup>25,26</sup></p> <p>Containing reactive materials such as YSZ-supported iron oxide or ceria</p> <p>Energy transfer efficiency from solar to chemical (stored in CO): 20%</p> <p>Efficiency of CO<sub>2</sub> to CO: 25%</p>
Electrolyzer for CO <sub>2</sub> reduction (Elec.)		-	1-30	<p>Requiring significant energy input.</p> <p>Containing heterogeneous electrocatalysts for specific products (i.e., Ag for CO, Cu or Ag for ethanol, Sn for formic acid. <sup>27-29</sup></p>
Cultivation and Harvesting of Microalgae (C&H)		Ambient	Ambient	<p>Algae growth in open pond system or closed photobioreactor (PBR) <sup>30,31</sup>.</p> $[a]\text{CO}_2 + [b]\text{nutrients} + \text{sunlight} \rightarrow [c]\text{O}_2 + \text{biomass}$

Lipid extraction (Extract.)		-	-	Lipid extraction was assumed at 90% efficiency <sup>30</sup> . Oil/solvent phase was separated from water and biomass. Then, solvent was separated in stripper and recycled. The lipid was at 99.5% purity.
Hydrotreating for oil upgrading (Hydrotr.)		350	35	Hydrogen consumption 1.5%wt of feed <sup>30</sup>
CO Pressure Swing Adsorption (CO-PSA)		60	9	CO-PSA yield at 90%. Operating up to at 9 bar <sup>32</sup> Adsorbent: Cu-Cu <sup>+</sup> /θ-Al <sub>2</sub> O <sub>3</sub> Adsorbent rate: 16.4 ton/ton of feed. Adsorbent lifetime of 2 years.
H <sub>2</sub> Pressure Swing Adsorption (H <sub>2</sub> -PSA)		30-35	15	H <sub>2</sub> PSA yield at 90%. Operating up to at 15 bar. <sup>17,33</sup> Adsorbent: zeolite 5A. Adsorbent requirement: 0.01 kmol/kg of feed.
CO <sub>2</sub> Absorption by monoethanolamine (CO <sub>2</sub> -MEA)		25-120	1-15	CO <sub>2</sub> -MEA for 90% of CO <sub>2</sub> recovery <sup>17,34,35</sup> Monoethanolamine(MEA): 23%



*Reverse water-gas shift (RWGS)*: converts CO<sub>2</sub> and H<sub>2</sub> into CO and H<sub>2</sub>O, using Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst in this study<sup>10,11</sup>. CO<sub>2</sub> and H<sub>2</sub> were mixed, heated, and compressed before entering into plug flow reactor (RPlug model). Since RWGS is equilibrium reaction, mixture gas of three components CO, CO<sub>2</sub>, and H<sub>2</sub> required further gas component separation (e.g., CO<sub>2</sub> absorption) or mixed with outsourcing H<sub>2</sub> for optimal stoichiometric number,  $SN=(H_2+CO_2)/(CO_2+CO)$ , for specific further synthesis (e.g., methanol synthesis, Fischer-Tropsch synthesis, or dimethyl ether synthesis). The simplified process flow diagram and kinetic expression are presented in Table S2.1 – S2.2.

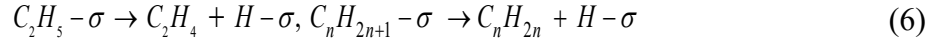
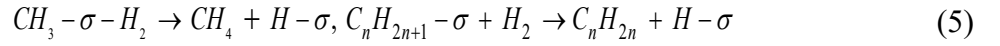
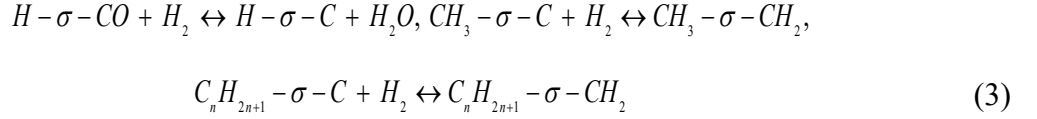
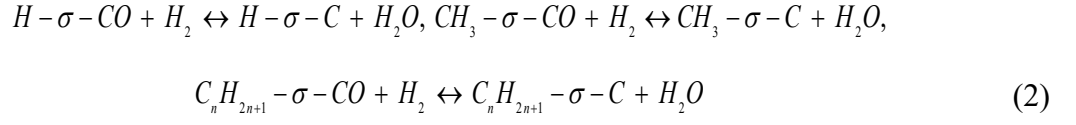
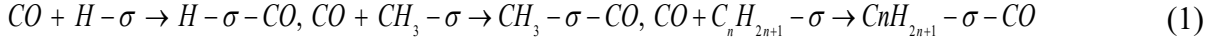
*Methanol synthesis*: MeOH is produced from syngas (mixture of CO and H<sub>2</sub>). In methanol synthesis unit, feed gas was first mixed with the recycle gas from downstream, before pressed up and heated to reaction condition. The RPlug model was used for plug flow reactor, that operated at 150 °C, 50 bar and filled by Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst<sup>25,36</sup>. In methanol synthesis unit, SN at 2 was preferred for optimal methanol yield. The kinetic expression and parameters are described in Table S2.1 – S2.2. Cooler and simple flash tank were operated right after reactor to separate liquid of methanol/water from unreacted gas that was further recycled back to reactor. The methanol/water liquid was brought into distillation column for purifying methanol from water.

**Table S2.2.** Kinetics and adsorption parameters for MS and RWGS reactions<sup>10</sup>

Parameters	Value
$k_1$	$1.07 \exp(36,696 \text{ kJkmol}^{-1}/RT)$
$k_2$	$1.22 \exp(-94,765 \text{ kJkmol}^{-1}/RT)$
$K_{e,1}$	$10^{(3,066/T - 10.592)}$
$K_{e,2}$	$10^{(-2073/T + 2.029)}$
	$6.62 \cdot 10^{-11} \exp(124,119 \text{ kJkmol}^{-1}/RT)$
	3,453.38

*Fischer-Tropsch synthesis (FTS)*: is the most common technology to produces liquid hydrocarbon (e.g., gasoline, diesel, and aviation fuels) from synthetic gas. Firstly, syngas was mixed with recycle stream (unreacted syngas), then pressed up and heated up to 38 bar and 210 °C before fed into reactor. The reaction mechanism was assumed by a series of reaction steps as shown in Eqs. (1) – (7)<sup>12</sup>. The kinetic expression and parameters are described in Table S2.1 and S2.3. The reactor outlet were brought to the separator unit, in which main hydrocarbon

products (i.e., FT fuels) flow out from the bottom while the light hydrocarbon gas, and unreacted gases are merged with steam and reformed before recycle <sup>12</sup>.



**Table S2.3.** Kinetics and adsorption parameters for FT reactions <sup>12</sup>

Parameters	Value	Unit	Parameters	Value	Unit
A <sub>1</sub>	1.83 x 10 <sup>9</sup>	kmol/kg <sub>cat</sub> ·h·bar	E <sub>1</sub>	1.00 x 10 <sup>5</sup>	kJ/kmol
A <sub>2</sub>	5.08	-	ΔH <sub>2</sub>	8.68 x 10 <sup>3</sup>	kJ/kmol
A <sub>3</sub>	2.44	1/bar	ΔH <sub>3</sub>	9.44 x 10 <sup>3</sup>	kJ/kmol
A <sub>4</sub>	2.90	-	ΔH <sub>4</sub>	7.90 x 10 <sup>3</sup>	kJ/kmol
A <sub>5</sub>	4.49 x 10 <sup>4</sup>	kmol/kg <sub>cat</sub> ·h·bar	E <sub>5</sub>	7.24 x 10 <sup>4</sup>	kJ/kmol
A <sub>5M</sub>	8.43 x 10 <sup>4</sup>	kmol/kg <sub>cat</sub> ·h·bar	E <sub>5M</sub>	6.30 x 10 <sup>4</sup>	kJ/kmol
A <sub>6</sub>	7.47 x 10 <sup>8</sup>	kmol/kg <sub>cat</sub> ·h·bar		9.72 x 10 <sup>4</sup>	kJ/kmol
A <sub>6E</sub>	7.03 x 10 <sup>8</sup>	kmol/kg <sub>cat</sub> ·h		1.09 x 10 <sup>5</sup>	kJ/kmol
A <sub>7</sub>	1.00 x 10 <sup>-4</sup>	1/bar	ΔH <sub>7</sub>	-2.50 x 10 <sup>5</sup>	kJ/kmol
			ΔE	1.12 x 10 <sup>3</sup>	kJ/kmol(CH <sub>2</sub> )

*Dimethyl ether synthesis (DMES)*: produces DME from syngas which is preferred CO/H<sub>2</sub> ratio at 1. Mixture feed gas was pressed up, and heated to 260 °C, 50 bar before fed in reactor filled catalyst of Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> and γ-Al<sub>2</sub>O<sub>3</sub> <sup>13</sup>. The outlet stream was brought into separation unit to separate DME from others (e.g., CO<sub>2</sub>, MeOH), and recycle unreacted H<sub>2</sub>/CO. In separation, chemical absorption using methanol for CO<sub>2</sub> absorption that results in liquid of DME/MeOH/CO<sub>2</sub>-rich solvent, and mixture of H<sub>2</sub>, CO (for recycling). The liquid stream then entered to two distillation columns for separating DME from CO<sub>2</sub>, and MeOH solvent, respectively. The simplified process flow diagram, kinetic expressions, and parameters for DMES are described in Table S2.1 and S2.4. Here, Rplug model was used for DMES reactor.

**Table S2.4.** Kinetics and parameters for dimethyl ether synthesis (DMES) <sup>13</sup>

Parameters	Value
$k_1$	$7,380 \exp(-54,307/RT)$
$k_2$	$5,059 \exp(-67,515/RT)$
$k_3$	$1,062 \exp(-43,473/RT)$
$k_4$	$7.3976 \exp(-20,436/RT)$
$K_{CO}$	$3.934 \times 10^{-6} \exp(37,373/RT)$
$K_{CO_2}$	$1.585 \times 10^{-6} \exp(53,795/RT)$
$K_{H_2}$	$0.6716 \exp(-6,476/RT)$
$K_{MeOH}$	$3.480 \times 10^{-6} \exp(54,689/RT)$

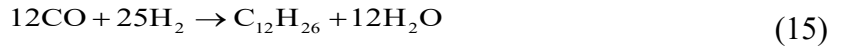
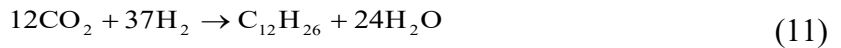
*Direct CO<sub>2</sub> hydrogenation to MeOH (DH-M):* directly synthesizes MeOH from CO<sub>2</sub> and H<sub>2</sub> in a single conversion pot, in which the two-step process of RWGS to CO and subsequent CO hydrogenation is proceeded. Firstly, CO<sub>2</sub> and H<sub>2</sub> was mixed with recycling, then pressed up and heated to 50 bar and 250 °C. Plug flow reactor was modeled using RPlug, in which kinetic expression for the catalyst of fibrous Cu/Zn/Al/Zr was embed as followed Table S2.1 and S2.5. <sup>15,37</sup>. Then, flash tank was operated for separating MeOH/water liquid, leaving gas of CO<sub>2</sub>, CO, H<sub>2</sub> for recycling. Finally, MeOH was separated and purified in distillation column.

**Table S2.5.** Kinetics and adsorption parameters for direct CO<sub>2</sub> hydrogenation to MeOH <sup>15,37</sup>

Parameters	Value	
$k_1$	$4.0638 \times 10^{-6} \exp(-11,695/RT)$	kmol/kg.s.Pa
$k_2$	$2.3714 \times 10^{-23} \exp(-112,860/RT)$	kmol/kg.s.Pa
$K_B$	$281.1780 \times \exp(-43,939/RT)$	-
$K_C$	$6.6687 \times 10^{-21} \exp(54,499/RT)$	Pa <sup>-2</sup>
$K_{CO}$	$8.3965 \times 10^{-11} \exp(118,270/RT)$	Pa <sup>-1</sup>
$K_{CO_2}$	$1.7214 \times 10^{-10} \exp(81,287/RT)$	Pa <sup>-1</sup>
$K_{H_2O}/K_H^{0.5}$	$4.3676 \times 10^{-12} \exp(956,775/RT)$	-

*Direct CO<sub>2</sub> hydrogenation to FT fuel (DH-FT):* Similarly to DH-M, the two-step process of RWGS to CO and subsequent CO hydrogenation is proceeded in one reactor. CO<sub>2</sub> and H<sub>2</sub> was first mixed with recycling, then pressed up and heated to 25 bar and 300 °C. DH-FT reactor contains Fe-based catalyst (here, Rstoic reactor model was used) that promotes reactions as shown in Eqs. (8) – (16) <sup>16</sup>. The following separation stage is similar to that of FTS. The main product of FT fuels was separated and purified from water, light gas and unreacted gas. The gas from the top of column was further treated in reforming unit that convert by-product C<sub>1</sub>-C<sub>4</sub> into syngas for recycling.





*Direct CO<sub>2</sub> hydrogenation to olefin (DH-O):* produces olefin (C<sub>2</sub>-C<sub>4</sub> hydrocarbon) from CO<sub>2</sub> and H<sub>2</sub> in one reactor filled by catalyst of Fe-K/γ-Al<sub>2</sub>O<sub>3</sub> and operated at 300 °C, 10 bar. RPlug reactor model was used, which embed kinetic metrics as shown in Table S2.6. Following separation target to separated olefin from liquid hydrocarbon (naphtha) as by-product, unreacted gas (CO<sub>2</sub>, H<sub>2</sub>) for recycling, and undesired gas (CO, CH<sub>4</sub>) for onsite heat and electricity generation. More description on DH-O can be found in Reference <sup>17</sup>.

**Table S2.6.** Kinetics and parameters for direct CO<sub>2</sub> hydrogenation to olefin <sup>17,18</sup>

No	Reaction	a <sub>i</sub>	b <sub>i</sub>	K <sub>0i</sub> (mol/(s.g.MPa))	E <sub>i</sub> (kJ/mol)
1	CO <sub>2</sub> +H <sub>2</sub> ↔ CO+H <sub>2</sub> O	53.4768	4.5679	0.619e8	136
2	CO+3H <sub>2</sub> → CH <sub>4</sub> +H <sub>2</sub> O	43.048	3.4174	0.3817e8	135
3	2CO+4H <sub>2</sub> → C <sub>2</sub> H <sub>4</sub> +2H <sub>2</sub> O	41.1777	3.1104	4.0918e8	146
4	2CO+5H <sub>2</sub> → C <sub>2</sub> H <sub>6</sub> +2H <sub>2</sub> O	85.9319	2.3182	0.4931e8	141
5	3CO+6H <sub>2</sub> → C <sub>3</sub> H <sub>6</sub> +3H <sub>2</sub> O	15.9468	4.0486	2.5451e8	147.1
6	3CO+7H <sub>2</sub> → C <sub>3</sub> H <sub>8</sub> +3H <sub>2</sub> O	55.5611	3.1525	0.0142e8	127
7	4CO+8H <sub>2</sub> → C <sub>4</sub> H <sub>8</sub> +4H <sub>2</sub> O	30.9118	4.9477	0.0014e8	111
8	4CO+9H <sub>2</sub> → C <sub>4</sub> H <sub>10</sub> +4H <sub>2</sub> O	87.9118	3.7471	84.4447	87
9	nCO <sub>2</sub> +3nH <sub>2</sub> → (CH <sub>2</sub> ) <sub>n</sub> +2nH <sub>2</sub> O	74.347	62.0165	36.5745	150

## S2.2. Simulation of CO<sub>2</sub>-to-fuel pathway

As proposed in CCU4E superstructure, there are 72 pathways for various fuel product from CO<sub>2</sub>. The process simulation of each pathway was performed in Aspen Plus software. In this part, we would present the simplified process flow diagram with stream information of some CO<sub>2</sub>-to-fuel pathways. Noted that the pathway number and integrated technologies for each was already presented in Table 1 in manuscript.

### S2.2.1. CO<sub>2</sub>-to-MeOH

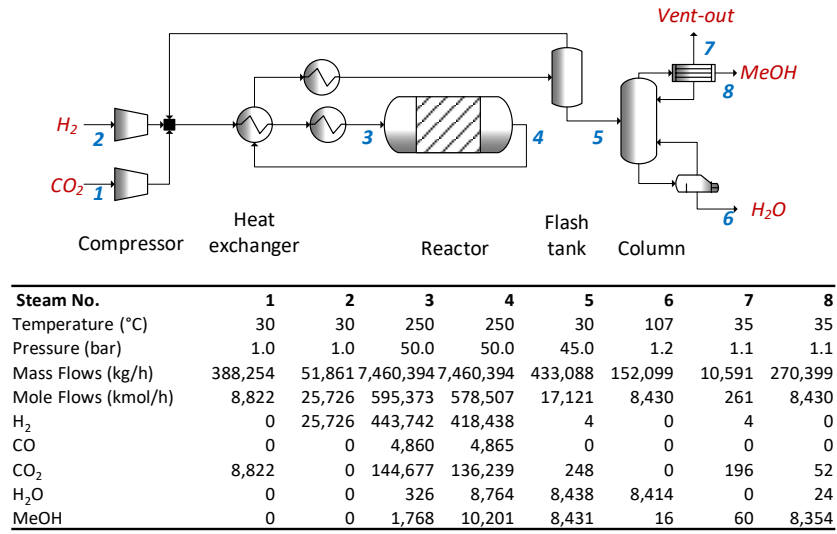


Fig. S2.2. Pathway #10 for methanol: Catalytic direct CO<sub>2</sub> hydrogenation to methanol

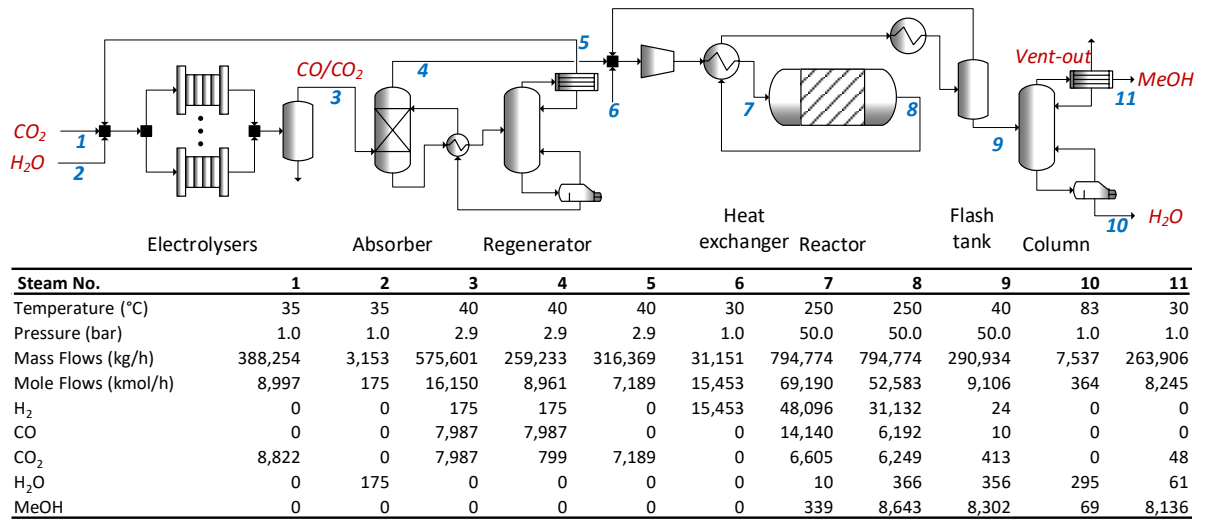
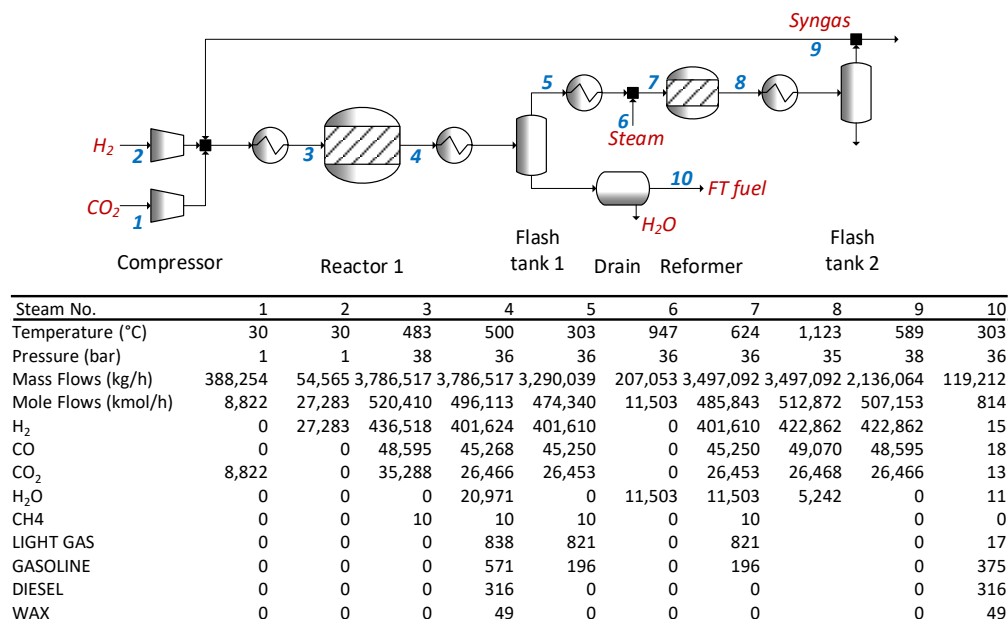


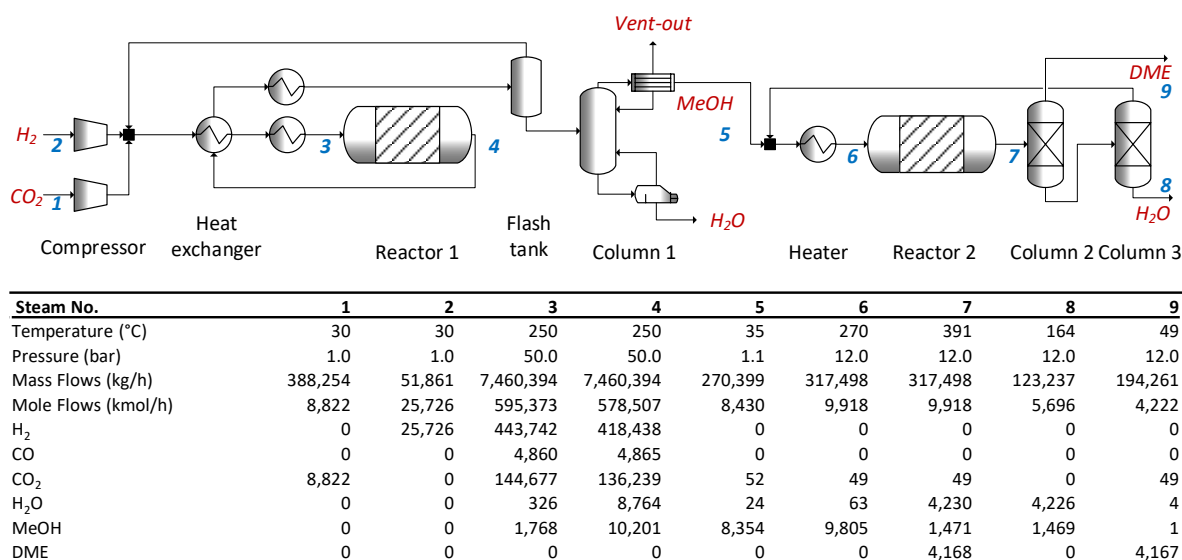
Fig. S2.3. Pathway #9 for methanol: Electrochemical CO<sub>2</sub> reduction to CO → CO<sub>2</sub>MEA → MeOH synthesis

### S2.2.2. CO<sub>2</sub>-to-FT fuels

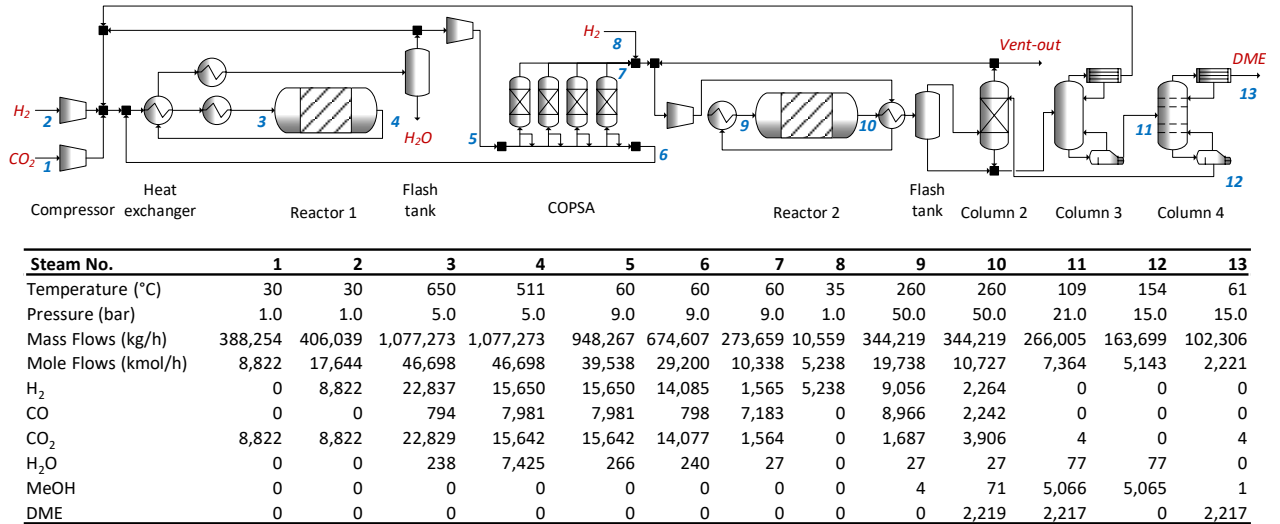


**Fig. S2.4.** Pathway #17 for FT fuels: Catalytic direct CO<sub>2</sub> hydrogenation to FT fuel

### S2.2.3. CO<sub>2</sub>-to-DME

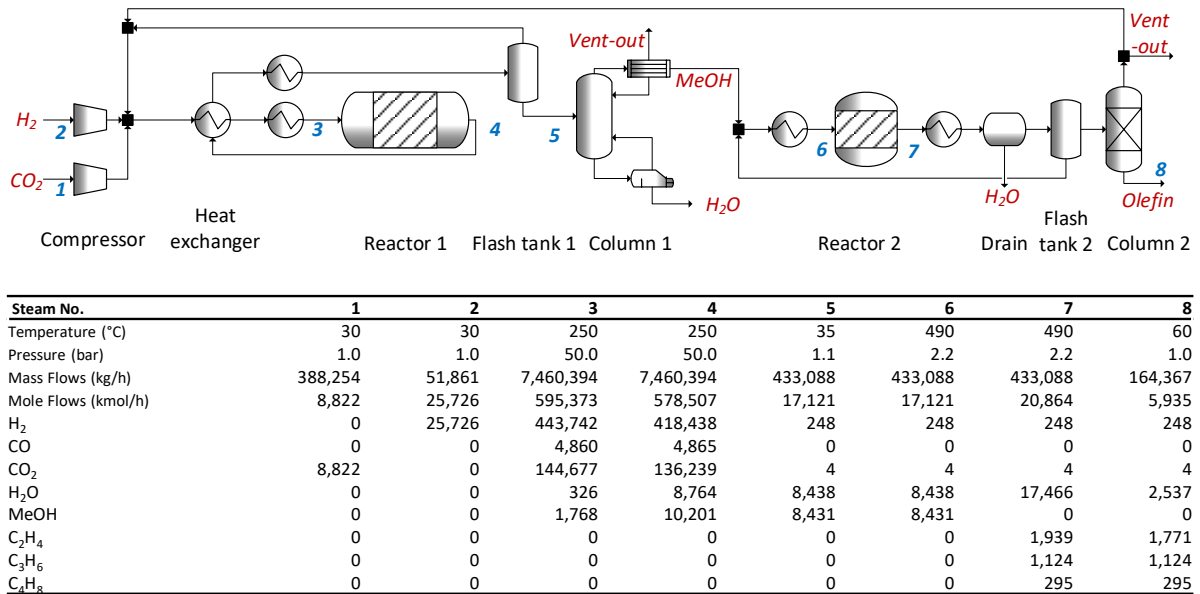


**Fig. S2.5.** Pathway #27 for dimethyl ether: Catalytic direct CO<sub>2</sub> hydrogenation to MeOH → Dehydration of MeOH to DME



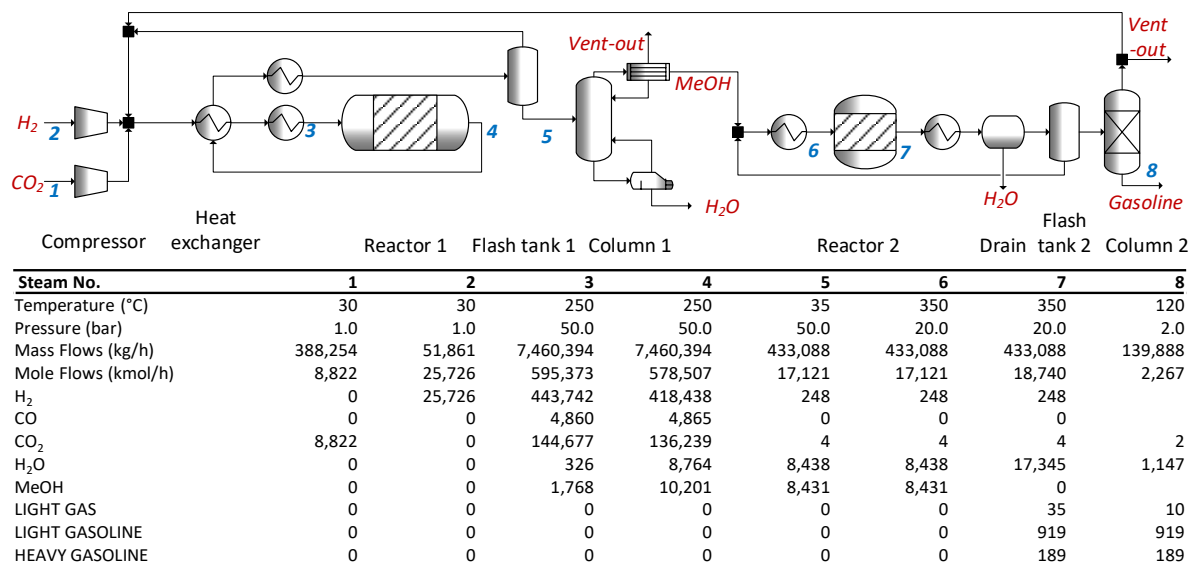
**Fig. S2.6.** Pathway #28 for dimethyl ether: Catalytic RWGS → COPSA → DME synthesis → Separation

### S2.2.4. CO<sub>2</sub>-to-olefin



**Fig. S2.7.** Pathway #43 for olefin: Catalytic direct CO<sub>2</sub> hydrogenation to MeOH → Methanol-to-olefin

### S2.2.4. CO<sub>2</sub>-to-gasoline



**Fig. S2.8.** Pathway #54 for gasoline: Catalytic direct CO<sub>2</sub> hydrogenation to MeOH → Methanol-to-gasoline



### S3. Economic, unit cost and CO<sub>2eq</sub> inventory assumptions

The economic parameters and cost of materials and utilities used in this study are presented in Table S3.1. Otherwise, The CO<sub>2eq</sub> inventory of raw material, conventional utility, and conventional fuels are presented in Table S3.2. Noted that using different raw material and utility sources (e.g., conventional or renewable based utility and H<sub>2</sub> feedstock) results in different Operating Cost (TOC) and indirect CO<sub>2</sub> emission (ICE).

**Table S3.1.** Economic assumptions and parameters

	Value	Unit	Ref.
<b>General parameters:</b>			
Reference year	2018		
Economic plant life	20	years	
Interest rate	8	%	
Operability	8000	h/y	
Scaling exponent	0.67	-	
Capacity Charge Factor (CCF)	0.1019	-	
<b>Total capital investment cost (TCI)</b>	<b>373</b>	<b>% of PE</b>	38
Direct plant cost (DC)	247	% of PE	
Purchased equipment (PE)	100	% of PE	
Equipment setting	39	% of PE	
Instrumentation and control	26	% of PE	
Piping	31	% of PE	
Electrical installation	10	% of PE	
Land	12	% of PE	
Building and building services	29	% of PE	
Indirect plant cost (IDC)	126	% of PE	
Engineering	32	% of PE	
Construction expenses	34	% of PE	
Contractor's fee	23	% of PE	
Contingency	37	% of PE	
Fixed operating cost (FOC)	5.1	% of TCI	20
<b>Materials and utilities:</b>			
<i>Raw material</i>			
Captured CO <sub>2</sub>	0.035	\$/kg	26
Renewable/green H <sub>2</sub>	4.415	\$/kg	39
Conventional/black H <sub>2</sub>	2.700	\$/kg	40
Process water	0.001	\$/kg	26
<i>Solvent, other materials input</i>			
Adsorbent for CO	50	\$/kg	32
Adsorbent for H <sub>2</sub>	6.11	\$/kg	17
<i>Conventional based utility</i>			
Electricity	0.060	\$/kWh	26
Low-pressure steam	0.014	\$/kWh	26
High-pressure steam	0.019	\$/kWh	26
Fired heat	0.029	\$/kWh	16
Cooling water	0.030	\$/ton	26
Refrigeration	0.063	\$/kWh	41
<i>Renewable based utility</i>			
RES-Electricity	0.073	\$/kWh	26
RES-Heat	0.050	\$/kWh	26
RES-Refrigeration	0.066	\$/kWh	41
<b>Market prices:</b>			
<i>Fuel products</i>			
Methanol	0.400	\$/kg	5

Ethanol	1.003	\$/kg	42
Olefin	0.673	\$/kg	43
Gasoline	0.847 <sup>a</sup>	\$/kg	44
Fischer-Tropsch fuel	1.173	\$/kg	5
Bio-diesel	1.000	\$/kg	45
Dimethyl ether	0.66	\$/kg	5
Formic acid	0.74	\$/kg	42
<i>By-products</i>			
Syngas (CO/H <sub>2</sub> )	0.550 <sup>b</sup>	\$/kg	
Naphtha	0.250	\$/kg	46
Electricity	0.073 <sup>c</sup>	\$/kg	

<sup>a</sup> Assumed at 2.5 \$/gal of gasoline  
<sup>b</sup> Estimated based on CO and H<sub>2</sub> price  
<sup>c</sup> Assumed at the same price of renewable electricity

**Table S3.2.** The CO<sub>2-eq</sub> inventory of raw material, conventional utility, and conventional fuels

	Value	Unit	Ref
<b>Raw material</b>			
Captured CO <sub>2</sub>	-1.00	kg/kg	
H <sub>2</sub> <sup>a</sup>	3.5	kg/kg	40
<b>Conventional utility</b>			
Electricity	0.6235	kg/kg	47
Low-pressure steam	0.1875	kg/kg	48
High-pressure steam	0.1875	kg/kg	48
Fuel gas	0.3406	kg/kg	48
Refrigeration	1.4746	kg/kg	48
<b>Fuel products</b>			
Methanol	0.300	kg/kg	49
Ethanol	1.923	kg/kg	50
Olefin	2.797	kg/kg	48
Gasoline	3.102	kg/kg	50
Fischer-Tropsch fuel	3.137	kg/kg	50
Biodiesel	0.039	kg/kg	48
Dimethyl ether	1.000	kg/kg	48
Formic acid	2.510	kg/kg	49

<sup>a</sup> Assumed produced via steam methane reforming with carbon capture and storage facility (SMRwCCS).

## S4. Techno-economic and environmental performance results (green H<sub>2</sub>)

### S.4.1. Mass, energy, and economic data of each technology

Based on process simulation, the mass balance, energy balance, and economic data was obtained for each technology as shown in Table S4.1 – S4.2. Then, the metrics for full CO<sub>2</sub>-to-fuel pathways, which is integration of technologies, were also estimated and obtained (shown in Table 1 of manuscript)

**Table S4.1.** Technical, economic and environment data of each technology obtained from simulation

Tech.	Group	Technology	Input	Output	Yield	CAP (kg/h)	TCI (M\$)	ER (kWh)	DCE (kg/h)
1	Catalytic conversion	RWGS 1	CO <sub>2</sub> , H <sub>2</sub>	CO <sub>2</sub> -rich 1	0.887	360,159	157.65	115,922	9
2		RWGS 2	CO <sub>2</sub> , H <sub>2</sub>	CO <sub>2</sub> -rich 4	0.682	277,032	257.76	298,149	39
3		RWGS 3	CO <sub>2</sub> , H <sub>2</sub>	CO <sub>2</sub> -rich 7	0.769	312,275	164.01	335,541	33
4		MS 1	CO <sub>2</sub> -rich 1	Raw MeOH 1	0.948	371,459	478.92	411,221	11,357
5		MS 2	CO <sub>2</sub> -rich 2	Raw MeOH 2	0.979	389,584	545.62	408,428	6,359
6		MS 3	CO <sub>2</sub> -rich 3	Raw MeOH 3	0.982	352,009	457.31	334,527	4,692
7		MS 4	Syngas 4	Raw MeOH 4	0.987	301,726	362.69	220,013	2,293
8		MS 5	Syngas 5	Raw MeOH 5	0.987	308,531	364.81	238,724	2,731
9		MS 6	Syngas 6	Raw MeOH 6	0.991	290,793	347.96	187,319	1,284
10		MS 7	Syngas 7	Raw MeOH 7	0.985	324,201	449.88	287,269	3,617
11		MS 8	Syngas 8	Raw MeOH 8	0.987	308,648	412.82	250,647	2,732
12		MS 9	Syngas 9	Raw MeOH 9	0.991	290,934	390.84	250,647	1,284
13		DHCO <sub>2</sub> -MeOH 1	CO <sub>2</sub> , H <sub>2</sub>	Raw MeOH 10	0.984	433,088	721.69	175,478	5,985
14		DMES 1	Syngas 4	Raw DME 11	0.999	283,924	293.09	75,996	27
15		DMES 2	Syngas 5	Raw DME 12	0.999	289,229	292.70	77,471	26
16		DMES 3	Syngas 6	Raw DME 13	1.00	273,684	298.83	83,888	30
17		DMES 4	Syngas 7	Raw DME 14	1.00	302,288	208.71	79,921	21
18		DMES 5	Syngas 8	Raw DME 15	1.00	289,342	292.75	77,515	26
19		DMES 6	Syngas 9	Raw DME 16	1.00	273,786	298.86	83,911	31
20		FTS 1	Syngas 4	FT fuel 1	0.27	82,312	798.27	900,087	3,211
21		FTS 2	Syngas 5	FT fuel 2	0.26	81,670	795.61	907,666	3,485
22		FTS 3	Syngas 6	FT fuel 3	0.28	83,605	782.62	859,714	2,912
23		FTS 4	Syngas 7	FT fuel 4	0.24	79,920	819.31	969,527	3,798
24		FTS 5	Syngas 8	FT fuel 5	0.26	81,706	795.72	908,017	3,486
25		FTS 6	Syngas 9	FT fuel 6	0.28	83,648	782.79	860,222	2,915
26		DHCO <sub>2</sub> -FT 1	CO <sub>2</sub> , H <sub>2</sub>	FT fuel 7	0.27	119,212	880.48	437,800	145,858
27		DHCO <sub>2</sub> -O 1	CO <sub>2</sub> , H <sub>2</sub>	Raw olefin 1	0.40	176,191	1,186.43	354,912	14,396
28	Thermochemical energizing	CR5 1	CO <sub>2</sub>	CO <sub>2</sub> -rich 2	0.91	352,968	10,356.30	26,370	

29		CR5 2	CO2	CO2-rich 5	0.72	280,796	31,403.34	114,700	
30		CR5 3	CO2	CO2-rich 8	0.72	280,796	31,403.34	111,481	
31	Electrochemical reduction	Elec-S 1	CO2	CO2-rich 3	0.81	318,034	2,754.12	434,017	
32		Elec-S 2	CO2	CO2-rich 6	0.67	260,815	4,986.99	785,906	
33		Elec-S 3	CO2	CO2-rich 9	0.66	259,233	4,986.99	805,328	
34		Elec-FA 1	CO2	Raw FA 1	0.67	361,486	15,640.50	1,676,735	1,885
35		Elec-FA	CO2	Raw EtOH 1	0.32	199,296	25,037.57	3,148,615	1,820
36	Separation	CO-PSA 1	CO2-rich 4	Syngas 4	0.98	273,659	2,991.53	18,601	3,098
37		CO-PSA 2	CO2-rich 5	Syngas 5	0.98	276,701	3,444.78	9,801	3,990
38		CO-PSA 3	CO2-rich 6	Syngas 6	0.99	259,093	1,930.97	45,231	1,582
39		CO2-MEA 1	CO2-rich 7	Syngas 7	0.95	298,114	32.41	841,185	6,001
40		CO2-MEA 2	CO2-rich 8	Syngas 8	0.99	276,806	30.19	756,388	3,990
41		CO2-MEA 3	CO2-rich 9	Syngas 9	1.00	259,233	28.61	698,303	1,582
42		SEP-MeOH 1	Raw MeOH 1	MeOH 1	0.67	249,861	27.75	231,946	25,372
43		SEP-MeOH 2	Raw MeOH 2	MeOH 2	0.65	253,538	32.28	243,792	26,479
44		SEP-MeOH 3	Raw MeOH 3	MeOH 3	0.73	255,491	31.25	221,899	25,680
45		SEP-MeOH 4	Raw MeOH 4	MeOH 4	0.86	259,415	26.76	170,773	21,073
46		SEP-MeOH 5	Raw MeOH 5	MeOH 5	0.83	256,482	27.59	203,507	22,470
47		SEP-MeOH 6	Raw MeOH 6	MeOH 6	0.91	264,255	24.82	150,303	15,911
48		SEP-MeOH 7	Raw MeOH 7	MeOH 7	0.78	253,149	45.47	235,083	24,186
49		SEP-MeOH 8	Raw MeOH 8	MeOH 8	0.83	256,594	27.59	203,566	22,477
50		SEP-MeOH 9	Raw MeOH 9	MeOH 9	0.91	263,906	23.82	118,289	16,073
51		SEP-MeOH 10	Raw MeOH 10	MeOH 10	0.62	270,399	11.90	207,718	8,643
52		SEP-DME 1	Raw DME 1	DME 1	0.72	179,506	38.93	150,381	
53		SEP-DME 2	Raw DME 2	DME 2	0.72	182,147	39.32	152,594	
54		SEP-DME 3	Raw DME 3	DME 3	0.72	183,550	39.52	153,769	
55		SEP-DME 4	Raw DME 4	DME 4	0.72	186,369	39.92	156,131	
56		SEP-DME 5	Raw DME 5	DME 5	0.72	184,262	39.62	154,366	
57		SEP-DME 6	Raw DME 6	DME 6	0.72	189,847	40.42	159,044	
58		SEP-DME 7	Raw DME 7	DME 7	0.72	181,868	39.27	152,360	
59		SEP-DME 8	Raw DME 8	DME 8	0.72	184,343	39.63	154,434	
60		SEP-DME 9	Raw DME 9	DME 9	0.72	189,596	40.39	158,834	
61		SEP-DME 10	Raw DME 10	DME 10	0.72	194,261	41.05	162,742	
62		SEP-DME 11	Raw DME 11	DME 11	0.36	102,306	30.45	118,378	178,987
63		SEP-DME 12	Raw DME 12	DME 12	0.33	95,613	29.58	113,076	179,711
64		SEP-DME 13	Raw DME 13	DME 13	0.42	113,816	33.45	125,712	157,457
65		SEP-DME 14	Raw DME 14	DME 14	0.27	80,462	28.58	98,047	209,859
66		SEP-DME 15	Raw DME 15	DME 15	0.33	95,667	44.23	103,671	191,668
67		SEP-DME 16	Raw DME 16	DME 16	0.42	113,886	33.45	125,699	157,493
68		SEP-O 1	Raw olefin 1	Olefin 11	0.39	68,270	1,213.90	133,589	24,791
69		SEP-FA 1	Raw FA 1	FA 1	0.99	359,366	63.29	11	42
70		SEP-EtOH 1	Raw EtOH 1	EtOH 1	0.24	47,900	203.04	22,254	

71	Upgrading	Dehydration 1	MeOH 1	Raw DME 1	1.00	249,858	547.00	82,171	
72		Dehydration 2	MeOH 2	Raw DME 2	1.00	253,535	552.38	83,380	
73		Dehydration 3	MeOH 3	Raw DME 3	1.00	255,488	555.23	84,022	
74		Dehydration 4	MeOH 4	Raw DME 4	1.00	259,412	560.93	85,313	
75		Dehydration 5	MeOH 5	Raw DME 5	1.00	256,479	556.67	84,348	
76		Dehydration 6	MeOH 6	Raw DME 6	1.00	264,252	567.92	86,904	
77		Dehydration 7	MeOH 7	Raw DME 7	1.00	253,146	551.82	83,252	
78		Dehydration 8	MeOH 8	Raw DME 8	1.00	256,591	556.84	84,385	
79		Dehydration 9	MeOH 9	Raw DME 9	1.00	263,903	567.42	86,789	
80		Dehydration 10	MeOH 10	Raw DME 10	1.00	270,396	576.73	88,925	
81		MTO 1	Raw MeOH 1	Olefin 1	0.38	140,552	4.03	0	
82		MTO 2	Raw MeOH 2	Olefin 2	0.38	147,410	4.23	0	
83		MTO 3	Raw MeOH 3	Olefin 3	0.38	133,193	3.82	0	
84		MTO 4	Raw MeOH 4	Olefin 4	0.38	114,167	3.28	0	
85		MTO 5	Raw MeOH 5	Olefin 5	0.38	116,741	3.35	0	
86		MTO 6	Raw MeOH 6	Olefin 6	0.38	110,030	3.16	0	
87		MTO 7	Raw MeOH 7	Olefin 7	0.38	122,671	3.52	0	
88		MTO 8	Raw MeOH 8	Olefin 8	0.38	116,786	3.35	0	
89		MTO 9	Raw MeOH 9	Olefin 9	0.38	110,083	3.16	0	
90		MTO 10	Raw MeOH 10	Olefin 10	0.38	163,871	4.70	0	
91		MTG 1	Raw MeOH 1	Gasoline 1	0.32	119,981	883.49	79	
92		MTG 2	Raw MeOH 2	Gasoline 2	0.32	125,836	912.15	83	
93		MTG 3	Raw MeOH 3	Gasoline 3	0.32	113,699	852.22	75	
94		MTG 4	Raw MeOH 4	Gasoline 4	0.32	97,458	768.61	65	
95		MTG 5	Raw MeOH 5	Gasoline 5	0.32	99,655	780.18	66	
96		MTG 6	Raw MeOH 6	Gasoline 6	0.32	93,926	749.83	62	
97		MTG 7	Raw MeOH 7	Gasoline 7	0.32	104,717	806.51	69	
98		MTG 8	Raw MeOH 8	Gasoline 8	0.32	99,693	780.37	66	
99		MTG 9	Raw MeOH 9	Gasoline 9	0.32	93,972	750.07	62	
100		MTG 10	Raw MeOH 10	Gasoline 10	0.32	139,888	979.19	93	
101		DTG 1	Raw DME 1	Gasoline 11	0.47	84,685	25.74	13,692	
102		DTG 2	Raw DME 2	Gasoline 12	0.47	85,931	25.99	13,894	
103		DTG 3	Raw DME 3	Gasoline 13	0.47	86,593	26.13	14,001	
104		DTG 4	Raw DME 4	Gasoline 14	0.47	87,923	26.39	14,216	
105		DTG 5	Raw DME 5	Gasoline 15	0.47	86,929	26.19	14,055	
106		DTG 6	Raw DME 6	Gasoline 16	0.47	89,563	26.72	14,481	
107		DTG 7	Raw DME 7	Gasoline 17	0.47	85,799	25.97	13,872	
108		DTG 8	Raw DME 8	Gasoline 18	0.47	86,967	26.20	14,061	
109		DTG 9	Raw DME 9	Gasoline 19	0.47	89,445	26.70	14,462	
110		DTG 10	Raw DME 10	Gasoline 20	0.47	91,646	27.14	14,818	
111		DTG 11	DME 11	Gasoline 21	0.47	48,265	17.66	7,804	
112		DTG 12	DME 12	Gasoline 22	0.47	45,107	16.88	7,293	

113		DTG 13	DME 13	Gasoline 23	0.47	53,694	18.97	8,682	
114		DTG 14	DME 14	Gasoline 24	0.47	37,959	15.04	6,137	
115		DTG 15	DME 15	Gasoline 25	0.47	45,133	16.88	7,297	
116		DTG 16	DME 16	Gasoline 26	0.47	53,728	18.98	8,687	

**Table S4.2.** Obtained input mass and energy, and by-product of each technology from process simulation

Tech.	Input materials											Input energy						By-product			
	CO <sub>2</sub> (kg/h)	H <sub>2</sub> (kg/h)	H <sub>2</sub> O (kg/h)	CO <sub>2</sub> - rich (kg/h)	Raw MeOH (kg/h)	MeOH (kg/h)	Raw DME (kg/h)	Raw olefin (kg/h)	Raw FA (kg/h)	Ads CO (kg/h)	Ads H <sub>2</sub> (kg/h)	LP (kWh)	HP (kWh)	FH (kWh)	Elec (kWh)	CW (ton/h)	REF (kWh)	Syngas (kg/h)	Light gas (kg/h)	Naphtha (kg/h)	Electricity (kg/h)
1	388,254	17,784												100,339	15,583	114,433					
2	388,254	17,784												272,916	25,233	53,262					
3	388,254	17,784												319,933	15,608	56,565					
4		31,834		360,159								290,025			121,196	88,583					
5		45,005		352,968								321,357			87,071	100,765					
6		40,313		318,034								252,302			82,225	83,200					
7		32,095		273,659								158,794			61,219	57,347					
8		35,894		276,701								175,763			62,961	61,804					
9		34,205		259,093								125,932			61,387	50,929					
10		31,151		298,114								208,395			78,874	70,998					
11		35,908		276,806								175,807			74,840	63,626					
12		34,207		259,233								175,807			74,840	63,626					
13	388,254	51,861												28,472	147,006	58,875					
14		10,559		273,659										21,619	41,928	11,061	12,449				
15		12,815		276,701										21,033	43,732	11,171	12,706				
16		14,928		259,093										22,703	48,804	12,323	12,381				
17		4,389		298,114										19,394	47,457	8,202	13,069				
18		12,823		276,806										21,044	43,756	11,178	12,715				
19		14,919		259,233										22,716	48,807	12,326	12,389				
20		36,451		273,659										780,859	119,228	118,337					
21		40,102		276,701										785,529	122,137	119,163					
22		37,618		259,093										742,448	117,266	112,331					
23		36,187		298,114										846,158	123,369	128,550					
24		40,118		276,806										785,831	122,186	119,208					
25		37,623		259,233										742,904	117,318	112,401					
26	388,254	54,565												273,443	164,358	67,850					
27	388,254	47,106								28		211,818			143,094	81,191				60,111	
28	388,254														26,370	5,864					
29	388,254														114,700	575,864					
30	388,254														111,481	19,428					



73						255,491							0	83,906	116	14,153							
74						259,415							0	85,194	118	14,370							
75						256,482							0	84,231	117	14,207							
76						264,255							0	86,784	120	14,638							
77						253,149							0	83,136	115	14,023							
78						256,594							0	84,268	117	14,214							
79						263,906								86,669	120	14,619							
80						270,399							0	88,802	123	14,978							
81					371,459								0			0							
82					389,584								0			0							
83					352,009								0			0							
84					301,726								0			0							
85					308,531								0			0							
86					290,793								0			0							
87					324,201								0			0							
88					308,648								0			0							
89					290,934								0			0							
90					433,088								0			0							
91					371,459											79							
92					389,584											83							
93					352,009											75							
94					301,726											65							
95					308,531											66							
96					290,793											62							
97					324,201											69							
98					308,648											66							
99					290,934											62							
100					433,088											93							
101						179,506							0	9	9,824	200	10,034	3,659				24,045	
102						182,147							0	9	9,969	203	10,181	3,713				24,399	
103						183,550							0	9	10,045	205	10,260	3,741				24,587	
104						186,369							0	9	10,200	208	10,417	3,799				24,965	
105						184,262							0	9	10,084	206	10,300	3,756				24,682	
106						189,847							0	9	10,390	212	10,612	3,870				25,430	
107						181,868							0	9	9,953	203	10,166	3,707				24,361	
108						184,343							0	9	10,089	206	10,304	3,758				24,693	
109						189,596							0	9	10,376	211	10,598	3,865				25,397	
110						194,261							0	10	10,632	217	10,859	3,960				26,022	
111						102,306							0	5	5,599	114	5,719	2,085				13,704	
112						95,613							0	5	5,233	107	5,344	1,949				12,808	
113						113,816							0	6	6,229	127	6,362	2,320				15,246	
114						80,462							0	4	4,404	90	4,498	1,640				10,778	



115							95,667					0	5	5,236	107	5,348	1,950		12,815		
116							113,886					0	6	6,233	127	6,366	2,321		15,255		

## S4.2. Techno-economic and environmental performance of full CO<sub>2</sub>-to-fuel pathways in CCU4E

Table S4.3 presents not only the integration of technologies involved each CO<sub>2</sub>-to-fuel pathway (from CO<sub>2</sub> feedstock to final fuel products), but also the estimated sizing and costing data for the techno-economic and environmental analysis.

**Table S4.3.** Techno-economic parameters of 72 CO<sub>2</sub>-to-fuel pathways

Pathway No.	Technology	Technology	Product	Yield	CAP (ton/h)	CAP (GGE/h)	ER (MWh)	DCE (ton/h)	TCI (M\$)	ACC (M\$)	FOC (M\$)	Credit (M\$)	Input materials				Input energy/utilities				
													CO <sub>2</sub> (ton/h)	H <sub>2</sub> (ton/h)	H <sub>2</sub> O (ton/h)	LPS (MWh)	HPS (MWh)	FH (MWh)	Elec (MWh)	CW (Mton/h)	Refr. (MWh)
1	Catalytic.	RWGS-MS-SEP	MeOH	0.57	249.9	47,376.8	759.1	36.7	664.3	67.7	33.9	0.0	388.3	49.6	0.0	231.9	290.0	100.3	136.8	0.2	0.0
2	Thermo.	CR5-MS-SEP	MeOH	0.59	253.5	48,074.0	678.6	32.8	10,934.2	1,113.7	557.6	0.0	388.3	45.0	0.0	243.8	321.4	0.0	113.4	0.1	0.0
3	Electro.	ELECZCO-MS-SEP	MeOH	0.59	255.5	48,444.3	990.4	30.4	3,242.7	330.3	165.4	0.0	388.3	40.3	3.2	221.9	252.3	0.0	516.2	0.1	0.0
4	Catalytic.	RWGS-COPSA-MS-SEP	MeOH	0.59	259.4	49,188.3	707.5	26.5	3,638.7	370.6	185.6	0.0	388.3	49.9	0.0	170.8	158.8	272.9	105.1	0.1	0.0
5	Thermo.	CR5-COPSA-MS-SEP	MeOH	0.60	256.5	48,632.2	566.7	29.2	35,240.5	3,589.3	1,797.3	0.0	388.3	35.9	0.0	203.5	175.8	0.0	187.5	0.7	0.0
6	Electro.	ELECZCO-COPSA-MS-SEP	MeOH	0.62	264.3	50,106.1	1,168.8	18.8	7,290.7	742.6	371.8	0.0	388.3	34.2	3.2	150.3	125.9	0.0	892.5	0.1	0.0
7	Catalytic.	RWGS-CO <sub>2</sub> MEA-MS-SEP	MeOH	0.58	253.1	48,000.2	1,699.1	33.8	691.8	70.5	35.3	0.0	388.3	48.9	0.0	1,076.0	208.4	319.9	94.8	0.3	0.0
8	Thermo.	CR5-CO <sub>2</sub> MEA-MS-SEP	MeOH	0.60	256.6	48,653.4	1,322.1	29.2	31,873.9	3,246.4	1,625.6	0.0	388.3	35.9	0.0	959.7	175.8	0.0	186.6	0.2	0.0
9	Electro.	ELECZCO-CO <sub>2</sub> MEA-MS-SEP	MeOH	0.62	263.9	50,039.9	1,872.6	18.9	5,430.3	553.1	276.9	0.0	388.3	34.2	3.2	816.3	175.8	0.0	880.4	0.2	0.0
10	Catalytic.	DHM-SEP	MeOH	0.61	270.4	51,271.0	383.2	14.6	733.6	74.7	37.4	0.0	388.3	51.9	0.0	207.7	0.0	28.5	147.0	0.1	0.0
11	Catalytic.	RWGS-COPSA-FTS-SEP	FT fuel	0.19	82.3	30,875.5	1,216.8	6.3	4,047.6	412.3	206.4	0.0	388.3	54.2	0.0	0.0	0.0	1,053.8	163.1	0.2	0.0
12	Thermo.	CR5-COPSA-FTS-SEP	FT fuel	0.19	81.7	30,634.7	1,032.2	7.5	35,643.7	3,630.4	1,817.8	0.0	388.3	40.1	0.0	0.0	0.0	785.5	246.6	0.7	0.0
13	Electro.	ELECZCO-COPSA-FTS-SEP	FT fuel	0.19	83.6	31,360.5	1,690.9	4.5	7,700.6	784.3	392.7	0.0	388.3	37.6	3.2	0.0	0.0	742.4	948.4	0.1	0.0
14	Catalytic.	RWGS-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	0.18	79.9	29,978.2	2,146.3	9.8	1,015.7	103.5	51.8	0.0	388.3	54.0	0.0	840.9	0.0	1,166.1	139.3	0.3	0.0
15	Thermo.	CR5-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	0.19	81.7	30,648.2	1,775.9	7.5	32,229.2	3,282.6	1,643.7	0.0	388.3	40.1	0.0	756.1	0.0	785.8	234.0	0.2	0.0
16	Electro.	ELECZCO-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	0.19	83.6	31,376.6	2,363.9	4.5	5,798.4	590.6	295.7	0.0	388.3	37.6	3.2	698.0	0.0	742.9	922.9	0.2	0.0
17	Catalytic.	DHFT-SEP	FT fuel	0.27	119.2	44,716.8	437.8	145.9	880.5	89.7	44.9	0.0	388.3	54.6	0.0	0.0	0.0	273.4	164.4	0.1	0.0
18	Catalytic.	RWGS-MS-DEHYDR-SEP	DME	0.41	179.5	46,911.3	991.6	36.7	1,250.3	127.3	63.8	0.0	388.3	49.6	0.0	231.9	440.4	182.4	136.9	0.3	0.0
19	Thermo.	CR5-MS-DEHYDR-SEP	DME	0.42	182.1	47,601.5	914.6	32.8	11,525.9	1,173.9	587.8	0.0	388.3	45.0	0.0	243.8	474.0	83.3	113.6	0.2	0.0
20	Electro.	ELECZCO-MS-DEHYDR-SEP	DME	0.43	183.6	47,968.1	1,228.2	30.4	3,837.4	390.8	195.7	0.0	388.3	40.3	3.2	221.9	406.1	83.9	516.4	0.2	0.0
21	Catalytic.	RWGS-COPSA-MS-DEHYDR-SEP	DME	0.43	186.4	48,704.8	949.0	26.5	4,239.6	431.8	216.2	0.0	388.3	49.9	0.0	170.8	314.9	358.1	105.2	0.2	0.0
22	Thermo.	CR5-COPSA-MS-DEHYDR-SEP	DME	0.43	184.3	48,154.2	805.4	29.2	35,836.8	3,650.1	1,827.7	0.0	388.3	35.9	0.0	203.5	330.1	84.2	187.6	0.7	0.0
23	Electro.	ELECZCO-COPSA-MS-DEHYDR-SEP	DME	0.45	189.8	49,613.8	1,414.7	18.8	7,899.1	804.5	402.9	0.0	388.3	34.2	3.2	150.3	285.0	86.8	892.6	0.1	0.0
24	Catalytic.	RWGS-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	0.42	181.9	47,528.6	1,934.7	33.8	1,282.9	130.7	65.4	0.0	388.3	48.9	0.0	1,076.0	360.8	403.1	94.9	0.3	0.0
25	Thermo.	CR5-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	0.43	184.3	48,175.4	1,560.9	29.2	32,470.4	3,307.2	1,656.0	0.0	388.3	35.9	0.0	959.7	330.2	84.3	186.7	0.3	0.0
26	Electro.	ELECZCO-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	0.45	189.6	49,548.2	2,118.2	18.9	6,038.1	615.0	307.9	0.0	388.3	34.2	3.2	816.3	334.6	86.7	880.5	0.2	0.0
27	Catalytic.	DHM-DEHYDR-SEP	DME	0.44	194.3	50,767.3	634.9	14.6	1,351.4	137.6	68.9	0.0	388.3	51.9	0.0	207.7	162.7	117.3	147.1	0.1	0.0
28	Catalytic.	RWGS-COPSA-DMES-SEP	DME	0.43	179.5	46,911.3	511.1	182.2	3,572.8	363.9	182.2	0.0	388.3	28.3	0.0	61.2	0.0	294.5	86.7	0.1	68.7
29	Thermo.	CR5-COPSA-DMES-SEP	DME	0.45	182.1	47,601.5	315.0	183.7	35,170.4	3,582.2	1,793.7	0.0	388.3	12.8	0.0	58.7	0.0	21.0	169.1	0.6	66.2
30	Electro.	ELECZCO-COPSA-DMES-SEP	DME	0.28	113.8	29,744.2	1,040.7	159.1	7,250.2	738.5	369.8	0.0	388.3	14.9	3.2	64.6	0.0	22.7	881.0	0.0	72.4
31	Catalytic.	RWGS-CO <sub>2</sub> MEA-DMES-SEP	DME	0.20	80.5	21,027.6	1,354.7	215.9	433.7	44.2	22.1	0.0	388.3	22.2	0.0	894.0	0.0	339.3	64.1	0.2	57.2
32	Thermo.	CR5-CO <sub>2</sub> MEA-DMES-SEP	DME	0.24	95.7	25,001.2	1,049.1	195.7	31,770.5	3,235.9	1,620.3	0.0	388.3	12.8	0.0	820.8	0.0	21.0	156.4	0.1	50.9
33	Electro.	ELECZCO-CO <sub>2</sub> MEA-DMES-SEP	DME	0.28	113.9	29,762.5	1,713.2	159.1	5,347.9	544.7	272.7	0.0	388.3	14.9	3.2	762.7	0.0	22.7	855.4	0.1	72.4
34	Catalytic.	RWGS-MS-MTO	Olefin	0.32	140.6	53,648.5	527.1	11.4	640.6	65.2	32.7	0.0	388.3	49.6	0.0	0.0	290.0	100.3	136.8	0.2	0.0
35	Thermo.	CR5-MS-MTO	Olefin	0.34	147.4	56,266.1	541.4	6.4	10,906.2	1,110.8	556.2	0.0	388.3	45.0	0.0	321.4	0.0	113.4	106.6	0.0	0.0

36	Electro.	ELECZCO-MS-MTO	Olefin	0.31	133.2	50,839.5	768.5	4.7	3,215.3	327.5	164.0	0.0	388.3	40.3	3.2	0.0	252.3	0.0	516.2	0.1	0.0
37	Catalytic.	RWGS-COPSA-MS-MTO	Olefin	0.26	114.2	43,577.3	536.8	5.4	3,615.3	368.2	184.4	0.0	388.3	49.9	0.0	0.0	158.8	272.9	105.1	0.1	0.0
38	Thermo.	CR5-COPSA-MS-MTO	Olefin	0.28	116.7	44,559.8	363.2	6.7	35,216.3	3,586.9	1,796.0	0.0	388.3	35.9	0.0	0.0	175.8	0.0	187.5	0.7	0.0
39	Electro.	ELECZCO-COPSA-MS-MTO	Olefin	0.26	110.0	41,998.3	1,018.5	2.9	7,269.1	740.4	370.7	0.0	388.3	34.2	3.2	0.0	125.9	0.0	892.5	0.1	0.0
40	Catalytic.	RWGS-CO <sub>2</sub> MEA-MS-MTO	Olefin	0.29	122.7	46,823.3	1,018.5	2.9	7,269.4	740.4	370.7	0.0	388.3	34.2	3.2	0.0	125.9	0.0	892.5	0.1	0.0
41	Thermo.	CR5-CO <sub>2</sub> MEA-MS-MTO	Olefin	0.28	116.8	44,577.0	1,118.5	6.7	31,849.7	3,244.0	1,624.3	0.0	388.3	35.9	0.0	756.1	175.8	0.0	186.6	0.2	0.0
42	Electro.	ELECZCO-CO <sub>2</sub> MEA-MS-MTO	Olefin	0.26	110.1	42,018.5	1,754.3	2.9	5,409.6	551.0	275.9	0.0	388.3	34.2	3.2	698.0	175.8	0.0	880.4	0.2	0.0
43	Catalytic.	DHM-MTO	Olefin	0.37	163.9	62,549.3	175.5	6.0	726.4	74.0	37.0	0.0	388.3	51.9	0.0	0.0	0.0	28.5	147.0	0.1	0.0
44	Catalytic.	DHO-SEP	Olefin	0.16	68.3	26,058.5	488.5	39.2	2,400.3	244.5	122.4	120.2	388.3	47.1	0.0	7.8	256.6	0.0	204.2	0.1	19.9
45	Catalytic.	RWGS-MS-MTG	Gasoline	0.27	120.0	45,895.5	527.2	11.4	1,520.1	154.8	77.5	0.0	388.3	49.6	0.0	0.0	290.0	100.3	136.9	0.2	0.0
46	Thermo.	CR5-MS-MTG	Gasoline	0.29	125.8	48,135.1	434.9	6.4	11,814.1	1,203.3	602.5	0.0	388.3	45.0	0.0	0.0	321.4	0.0	113.5	0.1	0.0
47	Electro.	ELECZCO-MS-MTG	Gasoline	0.26	113.7	43,492.4	768.6	4.7	4,063.7	413.9	207.2	0.0	388.3	40.3	3.2	0.0	252.3	0.0	516.3	0.1	0.0
48	Catalytic.	RWGS-COPSA-MS-MTG	Gasoline	0.22	97.5	37,279.9	536.8	5.4	4,380.6	446.2	223.4	0.0	388.3	49.9	0.0	0.0	158.8	272.9	105.1	0.1	0.0
49	Thermo.	CR5-COPSA-MS-MTG	Gasoline	0.23	99.7	38,120.3	363.3	6.7	35,993.1	3,666.0	1,835.6	0.0	388.3	35.9	0.0	0.0	175.8	0.0	187.5	0.7	0.0
50	Electro.	ELECZCO-COPSA-MS-MTG	Gasoline	0.22	93.9	35,928.8	1,018.5	2.9	8,015.8	816.4	408.8	0.0	388.3	34.2	3.2	0.0	125.9	0.0	892.6	0.1	0.0
51	Catalytic.	RWGS-CO <sub>2</sub> MEA-MS-MTG	Gasoline	0.24	104.7	40,056.6	1,464.1	9.7	1,452.8	148.0	74.1	0.0	388.3	48.9	0.0	840.9	208.4	319.9	94.9	0.2	0.0
52	Thermo.	CR5-CO <sub>2</sub> MEA-MS-MTG	Gasoline	0.24	99.7	38,134.8	1,118.6	6.7	32,626.7	3,323.1	1,664.0	0.0	388.3	35.9	0.0	756.1	175.8	0.0	186.7	0.2	0.0
53	Electro.	ELECZCO-CO <sub>2</sub> MEA-MS-MTG	Gasoline	0.22	94.0	35,946.4	1,754.3	2.9	6,156.5	627.1	314.0	0.0	388.3	34.2	3.2	698.0	175.8	0.0	880.5	0.2	0.0
54	Catalytic.	DHM-MTG	Gasoline	0.32	139.9	53,510.3	175.6	6.0	1,700.9	173.2	86.7	0.0	388.3	51.9	0.0	0.0	0.0	28.5	147.1	0.1	0.0
55	Catalytic.	RWGS-MS-DEHYDR-SEP-DTG	Gasoline	0.19	84.7	32,393.9	1,005.3	36.7	1,276.0	130.0	65.1	48.1	388.3	49.6	0.0	231.9	440.4	192.2	137.1	0.3	3.7
56	Thermo.	CR5-MS-DEHYDR-SEP-DTG	Gasoline	0.20	85.9	32,870.6	928.5	32.8	11,551.9	1,176.6	589.1	48.8	388.3	45.0	0.0	243.8	474.0	93.2	113.8	0.2	3.7
57	Electro.	ELECZCO-MS-DEHYDR-SEP-DTG	Gasoline	0.20	86.6	33,123.7	1,242.2	30.4	3,863.5	393.5	197.0	49.2	388.3	40.3	3.2	221.9	406.1	94.0	516.6	0.2	3.7
58	Catalytic.	RWGS-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	0.20	87.9	33,632.5	963.2	26.5	4,266.0	434.5	217.6	49.9	388.3	49.9	0.0	170.8	314.9	368.3	105.4	0.2	3.8
59	Thermo.	CR5-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	0.20	86.9	33,252.2	819.5	29.2	35,863.0	3,652.7	1,829.0	49.4	388.3	35.9	0.0	203.5	330.1	94.3	187.8	0.7	3.8
60	Electro.	ELECZCO-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	0.21	89.6	34,260.0	1,429.2	18.8	7,925.8	807.3	404.2	50.9	388.3	34.2	3.2	150.3	285.0	97.2	892.9	0.1	3.9
61	Catalytic.	RWGS-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	0.20	85.8	32,820.1	1,948.6	33.8	1,308.8	133.3	66.8	48.7	388.3	48.9	0.0	1,076.0	360.8	413.0	95.1	0.3	3.7
62	Thermo.	CR5-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	0.21	87.0	33,266.8	1,575.0	29.2	32,496.6	3,309.9	1,657.3	49.4	388.3	35.9	0.0	959.7	330.2	94.4	186.9	0.3	3.8
63	Electro.	ELECZCO-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	0.21	89.4	34,214.7	2,132.7	18.9	6,064.8	617.7	309.3	50.8	388.3	34.2	3.2	816.3	334.7	97.0	880.8	0.2	3.9
64	Catalytic.	DHCO <sub>2</sub> MEOH-DEHYDR-SEP-DTG	Gasoline	0.21	91.6	35,056.5	649.7	14.6	1,378.5	140.4	70.3	52.0	388.3	51.9	0.0	207.7	162.8	127.9	147.3	0.1	4.0
65	Catalytic.	RWGS-COPSA-DMES-SEP-DTG	Gasoline	0.12	48.3	18,462.3	518.9	182.2	3,590.5	365.7	183.1	27.4	388.3	28.3	0.0	61.2	0.0	300.1	86.8	0.1	70.8
66	Thermo.	CR5-COPSA-DMES-SEP-DTG	Gasoline	0.11	45.1	17,254.4	322.3	183.7	35,187.3	3,583.9	1,794.6	25.6	388.3	12.8	0.0	58.7	0.0	26.3	169.2	0.6	68.2
67	Electro.	ELECZCO-COPSA-DMES-SEP-DTG	Gasoline	0.13	53.7	20,539.3	1,049.4	159.1	7,269.2	740.4	370.7	30.5	388.3	14.9	3.2	64.6	0.0	28.9	881.1	0.0	74.8
68	Catalytic.	RWGS-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	0.09	38.0	14,520.3	1,360.8	215.9	448.8	45.7	22.9	21.6	388.3	22.2	0.0	894.0	0.0	343.7	64.2	0.2	58.9
69	Thermo.	CR5-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	0.11	45.1	17,264.3	1,056.4	195.7	31,787.4	3,237.6	1,621.2	25.6	388.3	12.8	0.0	820.8	0.0	26.3	156.5	0.1	52.8
70	Electro.	ELECZCO-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	0.13	53.7	20,552.0	1,721.9	159.1	5,366.9	546.6	273.7	30.5	388.3	14.9	3.2	762.7	0.0	28.9	855.5	0.1	74.8
71	Electro.	ELECZFA-SEP	FA	0.66	359.4	15,701.9	1,676.7	1.9	15,703.8	1,599.5	800.9	0.0	388.3	0.0	154.7	0.0	0.0	1,676.7	0.0	0.0	0.0
72	Electro.	ELECZETOH-SEP	EtOH	0.08	47.9	11,728.2	3,170.9	1.8	25,240.6	2,570.8	1,287.3	658.1	388.3	0.0	233.1	0.0	0.0	0.0	3,152.9	0.0	17.9

Yield: calculated based on the main fuel product and material input.

CAP (ton/h or GGE/h): the capacity or production rate of each process.

ER (MWh): energy requirement that is energy required for process.

DCE (ton/h): direct CO<sub>2eq</sub> emission that was the CO<sub>2eq</sub> flow emit to the environment via vent-out gas, purge gas (obtained from process simulation).

TCI (M\$): total capital investment cost of plant.

ACC (M\$/y): annualized capital investment cost.

FOC (M\$/y): fixed operating cost (5.1 % of TCI).

Credit (M\$/y): achieved credits by byproducts (e.g., naphtha, extra-electricity,...)

Consumed utilities included low-pressure steam (LPS), high-pressure steam (HPS), fired heat (FH), electricity (Elec), cooling water (CW), refrigeration (Refri.).

#### **Technology abbreviations:**

Catalytic.: Catalytic CO<sub>2</sub> conversion, Thermo.: Thermochemical CO<sub>2</sub> energizing, Electro.: Electrochemical CO<sub>2</sub> reduction. RWGS: Reverse water-gas shift, DHM: Direct CO<sub>2</sub> hydrogenation to methanol, DHFT: Direct CO<sub>2</sub> hydrogenation to Fischer-Tropsch fuel, DHO: Direct CO<sub>2</sub> hydrogenation to light olefin, CR5: Thermochemical splitting via Counter-Rotating-Ring Receiver/Reactor/ Recuperator, ELECZCO: Electrochemical reduction to CO, ELECZETO: Electrochemical reduction to ethanol, ELECZefa: Electrochemical reduction to formic acid, MS: Methanol synthesis, FTS: Fischer-Tropsch synthesis, DMES: dimethylether synthesis, DEHYDR.: Dehydration of methanol to dimethylether, MTO: methanol-to-olefin, MTG: methanol-to-gasoline, DTG: DME-to-gasoline synthesis, COPSA: CO pressure swing adsorption, CO<sub>2</sub>MEA: CO<sub>2</sub> absorption by monoethanolamine, SEP: separation and purification.

**Table S4.4.** Energy flows in CO<sub>2</sub>-to-fuel pathways and energy efficiency of processes

Pathway No.	Material input (kWh)	Utility (kWh)	Product (kWh)	Energy efficiency	Pathway No.	Material input (kWh)	Utility (kWh)	Product (kWh)	Energy efficiency
1	1,954,949	759,090	1,596,334	58.82%	37	1,965,233	536,763	1,468,314	58.69%
2	1,773,197	678,590	1,619,826	66.07%	38	1,414,224	363,225	1,501,419	84.47%
3	1,588,332	990,442	1,632,304	63.30%	39	1,347,677	1,018,456	1,415,108	59.81%
4	1,965,233	707,536	1,657,374	62.01%	40	1,347,677	1,018,456	1,577,685	66.68%
5	1,414,224	566,732	1,638,635	82.72%	41	1,414,775	1,118,516	1,501,998	59.29%
6	1,347,677	1,168,759	1,688,296	67.09%	42	1,347,756	1,754,278	1,415,790	45.64%
7	1,928,039	1,699,077	1,617,341	44.59%	43	2,043,323	175,478	2,107,563	94.99%
8	1,414,775	1,322,082	1,639,351	59.90%	44	1,855,976	488,501	878,028	37.45%
9	1,347,756	1,872,567	1,686,066	52.36%	45	1,954,949	527,223	1,546,422	62.30%
10	2,043,323	383,196	1,727,549	71.19%	46	1,773,197	434,881	1,621,886	73.45%
11	2,136,859	1,216,837	1,040,332	31.02%	47	1,588,332	768,619	1,465,454	62.18%
12	1,580,019	1,032,166	1,032,218	39.52%	48	1,965,233	536,828	1,256,125	50.20%
13	1,482,149	1,690,850	1,056,674	33.30%	49	1,414,224	363,291	1,284,442	72.26%
14	2,126,457	2,146,253	1,010,100	23.64%	50	1,347,677	1,018,518	1,210,602	51.16%
15	1,580,649	1,775,886	1,032,673	30.77%	51	1,928,039	1,464,064	1,349,686	39.79%
16	1,482,346	2,363,853	1,057,218	27.49%	52	1,414,775	1,118,582	1,284,932	50.72%
17	2,149,861	437,801	1,506,707	58.23%	53	1,347,756	1,754,340	1,211,195	39.04%
18	1,954,949	991,641	1,580,650	49.07%	54	2,043,323	175,571	1,803,001	81.26%
19	1,773,197	914,563	1,603,906	54.59%	55	1,954,949	1,005,333	1,091,494	36.87%
20	1,588,332	1,228,234	1,616,260	52.50%	56	1,773,197	928,457	1,107,556	41.00%
21	1,965,233	948,979	1,641,083	51.52%	57	1,588,332	1,242,235	1,116,086	39.43%
22	1,414,224	805,445	1,622,529	66.87%	58	1,965,233	963,195	1,133,229	38.70%
23	1,347,677	1,414,707	1,671,708	55.36%	59	1,414,224	819,500	1,120,416	50.16%
24	1,928,039	1,934,689	1,601,449	37.93%	60	1,347,677	1,429,188	1,154,373	41.57%
25	1,414,775	1,560,899	1,623,243	49.90%	61	1,928,039	1,948,561	1,105,854	28.53%
26	1,347,756	2,118,190	1,669,498	44.07%	62	1,414,775	1,574,960	1,120,906	37.49%
27	2,043,323	634,863	1,710,576	58.43%	63	1,347,756	2,132,652	1,152,846	33.12%
28	1,116,714	511,125	1,580,650	88.83%	64	2,043,323	649,681	1,181,211	43.86%
29	504,911	315,049	1,603,906	93.93%	65	1,116,714	518,929	622,078	38.03%
30	588,163	1,040,736	1,002,213	56.29%	66	504,911	322,342	581,379	70.28%
31	873,616	1,354,693	708,513	29.09%	67	588,163	1,049,418	692,062	42.26%
32	505,226	1,049,054	842,401	49.58%	68	873,616	1,360,830	489,255	21.90%
33	587,809	1,713,242	1,002,830	39.87%	69	505,226	1,056,351	581,711	37.25%
34	1,954,949	527,144	1,807,655	72.83%	70	587,809	1,721,929	692,488	29.98%
35	1,773,197	541,427	1,895,856	81.91%	71	0	1,676,745	529,067	31.55%
36	1,588,332	768,543	1,713,010	72.68%	72	0	3,170,868	395,175	12.46%

Carbon and energy efficiency present how much carbon and energy are captured and stored in the products, which are expressed as follow:

$$\text{Carbon efficiency} = \frac{\text{Carbon in products}}{\text{Carbon in raw material}}, (\%) \quad (17)$$

$$\text{Energy efficiency} = \frac{\text{Heat of reaction of products}}{\text{Heat of reaction in raw material} + \text{Consumed energy as utility}}, (\%) \quad (18)$$

Fig. S4.1. ranks CO<sub>2</sub>-to-fuel pathways in terms of carbon efficiency, energy efficiency, unit production cost (UPC), and net CO<sub>2</sub>eq emission (NCE), in which the order is from good performance to bad performance.

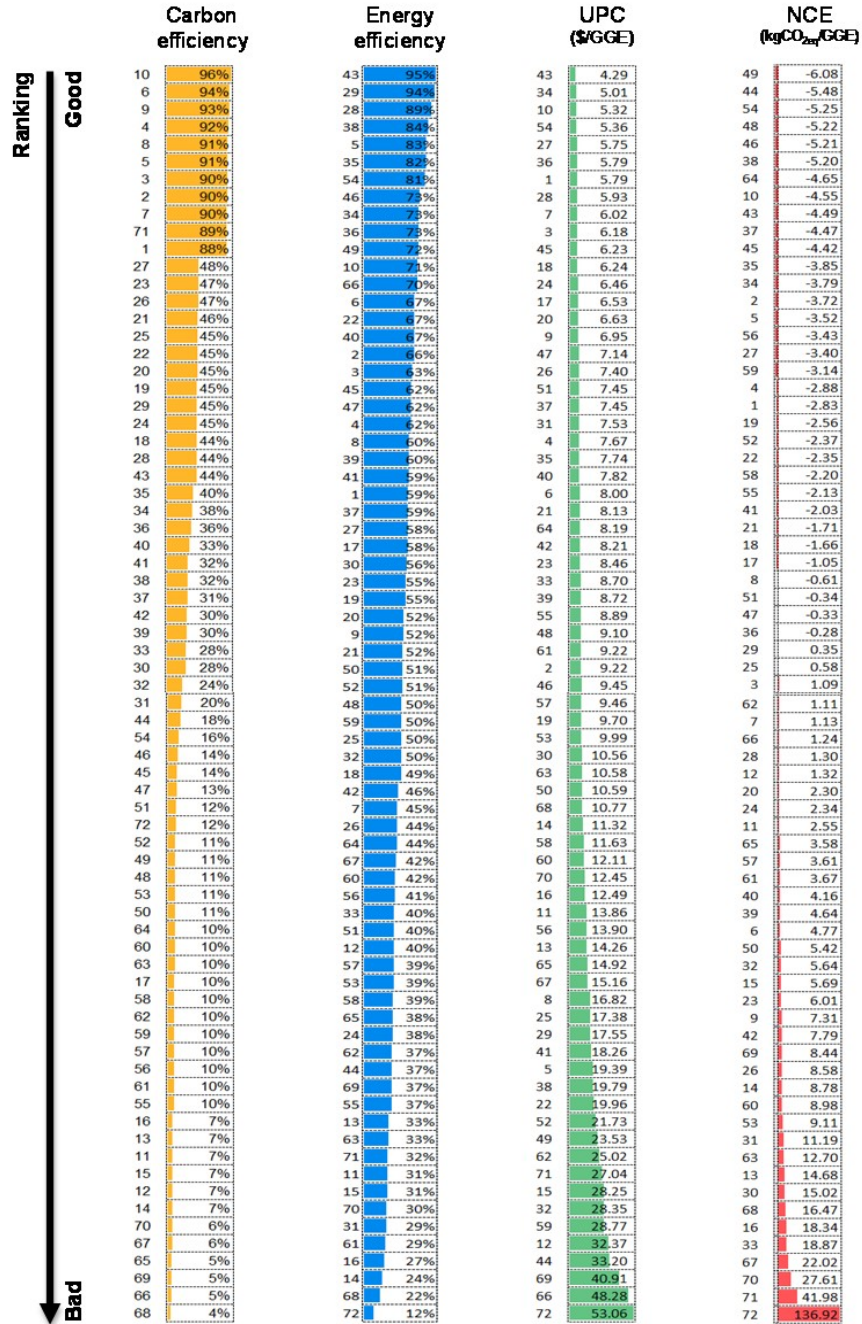


Fig. S4.1. Ranking CO<sub>2</sub>-to-fuel pathways by technical, economic and environmental performance

**Table S4.5.** CO<sub>2</sub>-based fuel's unit production cost and its breakdown (using green H<sub>2</sub>).

Unit: \$/GGE

Pathway No.	Technology	Product	UPC	ACC	CO <sub>2</sub>	H <sub>2</sub>	Utility	FOC
1	RWGS-MS-SEP	MeOH	5.83	0.18	0.29	4.65	0.63	0.09
2	CR5-MS-SEP	MeOH	9.26	2.90	0.28	4.16	0.47	1.45
3	ELECZCO-MS-SEP	MeOH	6.22	0.85	0.28	3.69	0.96	0.43
4	RWGS-COPSA-MS-SEP	MeOH	7.71	0.94	0.28	4.50	1.52	0.47
5	CR5-COPSA-MS-SEP	MeOH	19.42	9.23	0.28	3.28	2.01	4.62
6	ELECZCO-COPSA-MS-SEP	MeOH	8.02	1.85	0.27	3.03	1.94	0.93
7	RWGS-CO <sub>2</sub> MEA-MS-SEP	MeOH	6.06	0.18	0.28	4.53	0.97	0.09
8	CR5-CO <sub>2</sub> MEA-MS-SEP	MeOH	16.85	8.34	0.28	3.28	0.78	4.18
9	ELECZCO-CO <sub>2</sub> MEA-MS-SEP	MeOH	6.98	1.38	0.27	3.04	1.60	0.69
10	DHM-SEP	MeOH	5.36	0.18	0.27	4.49	0.33	0.09
11	RWGS-COPSA-FTS-SEP	FT fuel	13.93	1.67	0.44	7.80	3.19	0.84
12	CR5-COPSA-FTS-SEP	FT fuel	32.43	14.81	0.44	5.81	3.94	7.42
13	ELECZCO-COPSA-FTS-SEP	FT fuel	14.30	3.13	0.43	5.33	3.85	1.57
14	RWGS-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	11.40	0.43	0.45	7.99	2.30	0.22
15	CR5-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	28.30	13.39	0.44	5.81	1.96	6.70
16	ELECZCO-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	12.53	2.35	0.43	5.32	3.25	1.18
17	DHFT-SEP	FT fuel	6.58	0.25	0.30	5.42	0.49	0.13
18	RWGS-MS-DEHYDR-SEP	DME	6.28	0.34	0.29	4.70	0.78	0.17
19	CR5-MS-DEHYDR-SEP	DME	9.74	3.08	0.29	4.20	0.63	1.54
20	ELECZCO-MS-DEHYDR-SEP	DME	6.66	1.02	0.28	3.73	1.12	0.51
21	RWGS-COPSA-MS-DEHYDR-SEP	DME	8.17	1.11	0.28	4.55	1.68	0.55
22	CR5-COPSA-MS-DEHYDR-SEP	DME	19.99	9.47	0.28	3.31	2.18	4.74
23	ELECZCO-COPSA-MS-DEHYDR-SEP	DME	8.49	2.03	0.27	3.06	2.11	1.01
24	RWGS-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	6.50	0.34	0.29	4.57	1.13	0.17
25	CR5-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	17.41	8.58	0.28	3.31	0.94	4.30
26	ELECZCO-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	7.43	1.55	0.27	3.07	1.76	0.78
27	DHM-DEHYDR-SEP	DME	5.79	0.34	0.27	4.54	0.48	0.17
28	RWGS-COPSA-DMES-SEP	DME	5.95	0.97	0.29	2.68	1.53	0.49
29	CR5-COPSA-DMES-SEP	DME	17.56	9.41	0.29	1.20	1.96	4.71
30	ELECZCO-COPSA-DMES-SEP	DME	10.58	3.10	0.46	2.23	3.24	1.55
31	RWGS-CO <sub>2</sub> MEA-DMES-SEP	DME	7.57	0.26	0.65	4.68	1.85	0.13
32	CR5-CO <sub>2</sub> MEA-DMES-SEP	DME	28.37	16.18	0.54	2.28	1.27	8.10
33	ELECZCO-CO <sub>2</sub> MEA-DMES-SEP	DME	8.72	2.29	0.46	2.23	2.60	1.15
34	RWGS-MS-MTO	Olefin	5.05	0.15	0.25	4.11	0.46	0.08
35	CR5-MS-MTO	Olefin	7.77	2.47	0.24	3.55	0.28	1.24
36	ELECZCO-MS-MTO	Olefin	5.82	0.81	0.27	3.52	0.82	0.40
37	RWGS-COPSA-MS-MTO	Olefin	7.50	1.06	0.31	5.08	0.52	0.53
38	CR5-COPSA-MS-MTO	Olefin	19.82	10.06	0.30	3.58	0.84	5.04
39	ELECZCO-COPSA-MS-MTO	Olefin	8.75	2.20	0.32	3.62	1.51	1.10
40	RWGS-CO <sub>2</sub> MEA-MS-MTO	Olefin	7.85	1.98	0.29	3.24	1.35	0.99
41	CR5-CO <sub>2</sub> MEA-MS-MTO	Olefin	18.29	9.10	0.30	3.58	0.76	4.55
42	ELECZCO-CO <sub>2</sub> MEA-MS-MTO	Olefin	8.24	1.64	0.32	3.61	1.84	0.82
43	DHM-MTO	Olefin	4.32	0.15	0.22	3.68	0.20	0.07
44	DHO-SEP	Olefin	33.28	1.15	0.51	7.89	23.14	0.58
45	RWGS-MS-MTG	Gasoline	6.27	0.42	0.30	4.80	0.54	0.21
46	CR5-MS-MTG	Gasoline	9.49	3.12	0.28	4.15	0.37	1.56
47	ELECZCO-MS-MTG	Gasoline	7.18	1.19	0.31	4.12	0.96	0.60
48	RWGS-COPSA-MS-MTG	Gasoline	9.16	1.50	0.36	5.94	0.61	0.75
49	CR5-COPSA-MS-MTG	Gasoline	23.56	12.02	0.36	4.18	0.99	6.02
50	ELECZCO-COPSA-MS-MTG	Gasoline	10.63	2.84	0.38	4.23	1.76	1.42
51	RWGS-CO <sub>2</sub> MEA-MS-MTG	Gasoline	7.50	0.46	0.34	5.42	1.04	0.23
52	CR5-CO <sub>2</sub> MEA-MS-MTG	Gasoline	21.77	10.89	0.36	4.18	0.88	5.45
53	ELECZCO-CO <sub>2</sub> MEA-MS-MTG	Gasoline	10.03	2.18	0.38	4.23	2.16	1.09
54	DHM-MTG	Gasoline	5.40	0.40	0.25	4.30	0.23	0.20
55	RWGS-MS-DEHYDR-SEP-DTG	Gasoline	8.95	0.49	0.41	6.66	1.14	0.25
56	CR5-MS-DEHYDR-SEP-DTG	Gasoline	13.96	4.42	0.41	6.00	0.92	2.21
57	ELECZCO-MS-DEHYDR-SEP-DTG	Gasoline	9.51	1.46	0.40	5.30	1.62	0.73
58	RWGS-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	11.69	1.59	0.40	6.48	2.43	0.80
59	CR5-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	28.81	13.64	0.41	4.76	3.17	6.83
60	ELECZCO-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	12.15	2.90	0.39	4.37	3.04	1.45
61	RWGS-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	9.27	0.50	0.41	6.49	1.63	0.25
62	CR5-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	25.07	12.35	0.41	4.76	1.38	6.18

63	ELECZCO-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	10.62	2.22	0.39	4.36	2.54	1.11
64	DHCO <sub>2</sub> MEOH-DEHYDR-SEP-DTG	Gasoline	8.24	0.49	0.38	6.42	0.71	0.25
65	RWGS-COPSA-DMES-SEP-DTG	Gasoline	14.99	2.45	0.73	6.73	3.86	1.22
66	CR5-COPSA-DMES-SEP-DTG	Gasoline	48.31	25.86	0.78	3.28	5.42	12.95
67	ELECZCO-COPSA-DMES-SEP-DTG	Gasoline	15.19	4.45	0.65	3.19	4.66	2.23
68	RWGS-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	10.83	0.39	0.92	6.67	2.66	0.19
69	CR5-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	40.94	23.34	0.78	3.28	1.85	11.68
70	ELECZCO-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	12.48	3.28	0.65	3.18	3.74	1.64
71	ELECZFA-SEP	FA	27.04	12.73	0.87	0.00	7.05	6.38
72	ELECZETOH-SEP	EtOH	53.06	24.20	1.02	0.00	15.70	12.12

Abbreviation: UPC: unit production cost, ACC: annualized capital cost, CO<sub>2</sub>, H<sub>2</sub>, Utility: variable operating costs including CO<sub>2</sub> and H<sub>2</sub>, utility cost, FOC: fixed operating cost.

**Table S4.6.** Net CO<sub>2eq</sub> emission (NCE) and its components (using green H<sub>2</sub>).

Unit: kgCO<sub>2eq</sub>/GGE

Pathway No.	Technology	Product	NCE	CO <sub>2</sub> feed	Direct emission	Indirect emission
1	RWGS-MS-SEP	MeOH	-2.83	-8.20	0.78	4.59
2	CR5-MS-SEP	MeOH	-3.72	-8.08	0.68	3.68
3	ELECZCO-MS-SEP	MeOH	1.09	-8.01	0.63	8.48
4	RWGS-COPSA-MS-SEP	MeOH	-2.88	-7.89	0.54	4.48
5	CR5-COPSA-MS-SEP	MeOH	-3.52	-7.98	0.60	3.87
6	ELECZCO-COPSA-MS-SEP	MeOH	4.77	-7.75	0.37	12.14
7	RWGS-CO <sub>2</sub> MEA-MS-SEP	MeOH	1.13	-8.09	0.70	8.52
8	CR5-CO <sub>2</sub> MEA-MS-SEP	MeOH	-0.61	-7.98	0.60	6.77
9	ELECZCO-CO <sub>2</sub> MEA-MS-SEP	MeOH	7.31	-7.76	0.38	14.69
10	DHM-SEP	MeOH	-4.55	-7.57	0.29	2.74
11	RWGS-COPSA-FTS-SEP	FT fuel	2.55	-12.57	0.21	14.92
12	CR5-COPSA-FTS-SEP	FT fuel	1.32	-12.67	0.24	13.75
13	ELECZCO-COPSA-FTS-SEP	FT fuel	14.68	-12.38	0.14	26.92
14	RWGS-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	8.78	-12.95	0.33	21.40
15	CR5-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	5.69	-12.67	0.24	18.12
16	ELECZCO-CO <sub>2</sub> MEA-FTS-SEP	FT fuel	18.34	-12.37	0.14	30.57
17	DHFT-SEP	FT fuel	-1.05	-8.68	3.26	4.37
18	RWGS-MS-DEHYDR-SEP	DME	-1.66	-8.28	0.78	5.83
19	CR5-MS-DEHYDR-SEP	DME	-2.56	-8.16	0.69	4.91
20	ELECZCO-MS-DEHYDR-SEP	DME	2.30	-8.09	0.63	9.76
21	RWGS-COPSA-MS-DEHYDR-SEP	DME	-1.71	-7.97	0.54	5.72
22	CR5-COPSA-MS-DEHYDR-SEP	DME	-2.35	-8.06	0.61	5.10
23	ELECZCO-COPSA-MS-DEHYDR-SEP	DME	6.01	-7.83	0.38	13.46
24	RWGS-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	2.34	-8.17	0.71	9.80
25	CR5-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	0.58	-8.06	0.61	8.03
26	ELECZCO-CO <sub>2</sub> MEA-MS-DEHYDR-SEP	DME	8.58	-7.84	0.38	16.03
27	DHM-DEHYDR-SEP	DME	-3.40	-7.65	0.29	3.96
28	RWGS-COPSA-DMES-SEP	DME	1.30	-8.28	3.88	5.69
29	CR5-COPSA-DMES-SEP	DME	0.35	-8.16	3.86	4.65
30	ELECZCO-COPSA-DMES-SEP	DME	15.02	-13.05	5.35	22.73
31	RWGS-CO <sub>2</sub> MEA-DMES-SEP	DME	11.19	-18.46	10.27	19.38
32	CR5-CO <sub>2</sub> MEA-DMES-SEP	DME	5.64	-15.53	7.83	13.34
33	ELECZCO-CO <sub>2</sub> MEA-DMES-SEP	DME	18.87	-13.05	5.35	26.57
34	RWGS-MS-MTO	Olefin	-3.79	-7.24	0.21	3.24
35	CR5-MS-MTO	Olefin	-3.85	-6.90	0.11	2.94
36	ELECZCO-MS-MTO	Olefin	-0.28	-7.64	0.09	7.26
37	RWGS-COPSA-MS-MTO	Olefin	-4.47	-8.91	0.12	4.32
38	CR5-COPSA-MS-MTO	Olefin	-5.20	-8.71	0.15	3.36
39	ELECZCO-COPSA-MS-MTO	Olefin	4.64	-9.24	0.07	13.81
40	RWGS-CO <sub>2</sub> MEA-MS-MTO	Olefin	4.16	-8.29	0.06	12.39
41	CR5-CO <sub>2</sub> MEA-MS-MTO	Olefin	-2.03	-8.71	0.15	6.53
42	ELECZCO-CO <sub>2</sub> MEA-MS-MTO	Olefin	7.79	-9.24	0.07	16.96
43	DHM-MTO	Olefin	-4.49	-6.21	0.10	1.62
44	DHO-SEP	Olefin	-5.48	-14.90	1.50	7.91
45	RWGS-MS-MTG	Gasoline	-4.42	-8.46	0.25	3.79
46	CR5-MS-MTG	Gasoline	-5.21	-8.07	0.13	2.72
47	ELECZCO-MS-MTG	Gasoline	-0.33	-8.93	0.11	8.49

48	RWGS-COPSA-MS-MTG	Gasoline	-5.22	-10.41	0.15	5.05
49	CR5-COPSA-MS-MTG	Gasoline	-6.08	-10.18	0.18	3.93
50	ELECZCO-COPSA-MS-MTG	Gasoline	5.42	-10.81	0.08	16.15
51	RWGS-CO <sub>2</sub> MEA-MS-MTG	Gasoline	-0.34	-9.69	0.24	9.11
52	CR5-CO <sub>2</sub> MEA-MS-MTG	Gasoline	-2.37	-10.18	0.18	7.63
53	ELECZCO-CO <sub>2</sub> MEA-MS-MTG	Gasoline	9.11	-10.80	0.08	19.83
54	DHM-MTG	Gasoline	-5.25	-7.26	0.11	1.90
55	RWGS-MS-DEHYDR-SEP-DTG	Gasoline	-2.13	-11.99	1.13	8.72
56	CR5-MS-DEHYDR-SEP-DTG	Gasoline	-3.43	-11.81	1.00	7.38
57	ELECZCO-MS-DEHYDR-SEP-DTG	Gasoline	3.61	-11.72	0.92	14.41
58	RWGS-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	-2.20	-11.54	0.79	8.56
59	CR5-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	-3.14	-11.68	0.88	7.66
60	ELECZCO-COPSA-MS-DEHYDR-SEP-DTG	Gasoline	8.98	-11.33	0.55	19.76
61	RWGS-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	3.67	-11.83	1.03	14.47
62	CR5-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	1.11	-11.67	0.88	11.90
63	ELECZCO-CO <sub>2</sub> MEA-MS-DEHYDR-SEP-DTG	Gasoline	12.70	-11.35	0.55	23.49
64	DHCO <sub>2</sub> MEOH-DEHYDR-SEP-DTG	Gasoline	-4.65	-11.08	0.42	6.01
65	RWGS-COPSA-DMES-SEP-DTG	Gasoline	3.58	-21.03	9.87	14.74
66	CR5-COPSA-DMES-SEP-DTG	Gasoline	1.24	-22.50	10.65	13.10
67	ELECZCO-COPSA-DMES-SEP-DTG	Gasoline	22.02	-18.90	7.74	33.18
68	RWGS-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	16.47	-26.74	14.87	28.34
69	CR5-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	8.44	-22.49	11.33	19.59
70	ELECZCO-CO <sub>2</sub> MEA-DMES-SEP-DTG	Gasoline	27.61	-18.89	7.74	38.75
71	ELECZFA-SEP	FA	41.98	-24.73	0.12	66.58
72	ELECZETOH-SEP	EtOH	136.92	-33.10	0.16	169.87

## S5. Optimization model for optimal pathway identification

To identify the optimal CO<sub>2</sub>-to-fuel pathway from an economic perspective, we developed a network optimization model using a mixed integer linear programming (MILP) technique based on the generated CCU4E superstructure along with associated parameters that was obtained through a process simulation.

**Objective function:** The object function identifies the optimal CO<sub>2</sub>-to-fuel pathway for each CO<sub>2</sub>-based fuel types, which produce fuel at minimum UPC among several pathways. This objective function is calculated by annual capital cost, operating cost, and annual production rate.

$$MinUPC_s = \sum_j X_{js} \left( \frac{\sum_j \alpha_j + \sum_j \psi_j + \sum_{i \in I^U} \varpi_i \gamma_{ij} + \sum_{i \in I^F} \xi_i F_{ij} - \sum_{i \in I^B} \pi_i S_{ij}}{\sum_{i \in I^P} S_{ij}} \right) \quad (17)$$

where  $X_{js}$  is the binary variable for the selection of pathway  $j$  in each fuel  $s$ ,  $\alpha_j$  is the total capital investment cost of pathway  $j$ ,  $\psi_j$  is the fixed operating cost factor of pathway  $j$ .  $\gamma_{ij}$  and  $F_{ij}$  is the amount of utilities and feestock, respectively.  $\varpi_i$  and  $\xi_i$  are the unit costs for utilities  $i \in I^U$  and feedstock  $i \in I^F$ , respectively.  $\delta_i$  is the annual production rate of final product  $i \in I^P$  and  $\pi_i$  is assumed unit price by-product  $i \in I^B$ .

### Constraints:

*Logistic constraints:* Only one pathway (the optimal one with the minimum UPC) should be selected toward each fuel  $s$ .

$$\sum_{j_1}^{j_n} X_{js} = 1$$

*Compound material balance:* the amount of feedstock and the production of a compound should be equal to the amount of product, by-product, and the consumption of compounds in pathway (a series of technologies):

$$F_i + \sum_{j \in J_i^+} \eta_{ij} Y_j = S_i - \sum_{j \in J_i^-} \eta_{ij} Y_j \quad \forall i \quad (18)$$



where  $F_i$  is the amount of feedstock  $i \in I^F$ ,  $\eta_{ij}$  is the yield of compound  $i$  in technology  $j$  ( $\eta_{ij} < 0$  for inputs and  $\eta_{ij} > 0$  for outputs),  $Y_j$  is the production level of technology  $j$ , and  $S_i$  is the amount of product  $i \in I^P$ , by-product  $i \in I^B$ .

*Capacity limits:* the total amount of the production each technology should be bounded by its capacity and the number of facilities:

$$Y_j \leq N_j \beta_j \quad (19)$$

where  $N_j$  is the number of technology  $j$ ,  $\beta_j$  is the capacity of technology  $j$ .

*Feed availability:* the amount of CO<sub>2</sub>  $i \in I^F$  for CO<sub>2</sub> utilization should be equal to its availability:

$$\sum_{i \in I^F} F_i = \rho \quad (20)$$

where  $\rho$  is the availability of CO<sub>2</sub>.

## S6. Analysis of CCU4E in different local scenarios

**Table S6.1.** Top country's share of CO<sub>2</sub> emissions <sup>51</sup>

	% in 2018	This study (Mt/y)
Global	100	1000
China	29	290
US	16	160
Europe	11	110
India	7	110
Japan	4	40
Korea	2	20
Rest of the world	31	270

**Table S6.2.** The unit price of black H<sub>2</sub> (estimated based on natural gas market) <sup>47,52-54</sup>

	Natural gas (\$/MMBTU)	Natural gas (\$/GJ)	Black H <sub>2</sub> * (\$/kg)
Global	4.38	4.15	2.7
USA	3.15	2.99	2.3
Europe	7.68	7.28	4.1
China	8.1	7.68	4.3
India	8.1	7.68	4.3
Japan	8.1	7.68	4.3
Korea	8.1	7.68	4.3

\* H<sub>2</sub> is assumed to produce via steam methane reforming integrated with CO<sub>2</sub> capture and storage <sup>40</sup>.

**Table S6.3.** UPC and NCE of CO<sub>2</sub>-based fuels using black/green H<sub>2</sub> by country

Product	Scenario	UPC (\$/GGE)						NCE (kgCO <sub>2</sub> /GGE)					
		China	USA	Europe	India	Japan	Korea	China	USA	Europe	India	Japan	Korea
MeOH	Black H <sub>2</sub>	5.37	3.15	5.14	5.33	5.31	5.34	0.00	-1.23	-0.11	0.19	-0.29	-0.26
	Green H <sub>2</sub>	4.87	4.41	6.58	4.07	9.52	7.42	-0.67	-4.77	-0.78	-0.48	-0.29	-0.93
FT fuel	Black H <sub>2</sub>	6.78	3.88	6.47	6.72	6.70	6.73	1.69	2.94	1.43	2.19	0.96	1.05
	Green H <sub>2</sub>	6.17	5.40	8.21	5.20	11.78	9.25	0.09	-1.33	-0.17	0.59	0.96	-0.56
DME	Black H <sub>2</sub>	5.86	3.55	5.62	5.81	5.80	5.83	0.31	-0.04	0.17	0.58	-0.09	-0.04
	Green H <sub>2</sub>	5.36	4.82	6.86	4.54	8.64	7.39	-0.62	-3.62	-0.77	-0.35	-0.09	-0.98
Olefin	Black H <sub>2</sub>	4.33	2.52	4.14	4.30	4.28	4.31	-0.29	-1.77	-0.46	0.03	-0.77	-0.71
	Green H <sub>2</sub>	3.92	3.54	5.32	3.26	7.74	6.01	-1.40	-4.67	-1.57	-1.08	-0.77	-1.82
Gasoline	Black H <sub>2</sub>	5.41	3.29	5.19	5.37	5.36	5.38	-0.34	-2.07	-0.54	0.04	-0.90	-0.84
	Green H <sub>2</sub>	4.93	4.49	6.57	4.16	9.39	7.38	-1.64	-5.46	-1.84	-1.26	-0.90	-2.13

## S7. Future estimation of black and green H<sub>2</sub>

Basically, green H<sub>2</sub> price was estimated based on the price of green electricity type (e.g., solar-based, wind-based, bioenergy) and technology development of water electrolyzer (e.g., alkaline – ALK, proton exchange membrane – PEM, solid oxide electrolyzer cell – SOEC). The price of various renewable-based electricity was assumed and estimated from references <sup>55–57</sup>, and presented in Table S7.1. Here, we also considered the potential development of electrolyzers with higher efficiency and lower capital cost, resulting in lower green H<sub>2</sub> price, in which the techno-economic characteristics was estimated and presented in Table S7. 2 – S7.4 <sup>55,58–60</sup>. Finally, green H<sub>2</sub> price was estimated and provided in Table S7.5.

**Table S7.1.** Estimated global renewable electricity price for 2020 – 2030

	Unit	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Solar Photovoltaic	\$/kWh	0.085	0.082	0.078	0.075	0.071	0.068	0.064	0.061	0.057	0.054	0.050
Onshore wind	\$/kWh	0.056	0.054	0.053	0.051	0.050	0.048	0.046	0.045	0.043	0.042	0.040
Offshore wind	\$/kWh	0.127	0.120	0.114	0.107	0.101	0.094	0.088	0.081	0.074	0.068	0.061
Concentrated solar panel	\$/kWh	0.185	0.177	0.168	0.160	0.151	0.143	0.134	0.126	0.117	0.109	0.100
Bioenergy	\$/kWh	0.062	0.062	0.062	0.061	0.061	0.061	0.061	0.061	0.060	0.060	0.060
Hydropower	\$/kWh	0.047	0.046	0.046	0.045	0.044	0.044	0.043	0.042	0.041	0.041	0.040
Geothermal	\$/kWh	0.072	0.071	0.071	0.070	0.069	0.069	0.068	0.067	0.066	0.066	0.065
Assumed for solar&wind	\$/kWh	0.071	0.068	0.065	0.063	0.060	0.058	0.055	0.053	0.050	0.048	0.045

**Table S7.2.** Assumption and estimated techno-economic characteristics for alkaline electrolyser (ALK) <sup>58</sup>

	Unit	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Efficiency (LHV)	%	67%	67%	67%	67%	67%	67%	67%	68%	68%	68%	68%
Efficiency	kWh/kgH <sub>2</sub>	50	50	50	50	50	50	49	49	49	49	49
Stack lifetime	Operating hours	80000	81000	82000	83000	84000	85000	86000	87000	88000	89000	90000
CAPEX	\$/kW	750	723	696	669	642	615	588	561	534	507	480
OPEX												
Stack replacement cost	\$/kW	340	723	696	669	642	615	588	561	534	507	215
Stack replacement	% of stack	10%	10%	10%	10%	10%	9%	9%	9%	9%	9%	9%
OPEX-FC	% of CAPEX	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%
Capacity	kWh	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000
Operability	h/y	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000

**Table S7.3.** Assumption and estimated techno-economic characteristics for proton exchange membrane electrolyser (PEM) <sup>58</sup>

	Unit	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Efficiency (LHV)	%	58%	59%	60%	60%	61%	62%	63%	63%	64%	65%	66%
Efficiency	kWh/kgH <sub>2</sub>	57	57	56	55	55	54	53	53	52	51	51
Stack lifetime	Operating hours	40000	43500	47000	50500	54000	57500	61000	64500	68000	71500	75000
CAPEX	\$/kW	1,200	1,150	1,100	1,050	1,000	950	900	850	800	750	700
OPEX												
Stack replacement cost	\$/kW	420	399	378	357	336	315	294	273	252	231	210
Stack replacement	% of stack	20%	18%	17%	16%	15%	14%	13%	12%	12%	11%	11%
OPEX-FC	% of CAPEX	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%
Capacity	kWh	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000
Operability	h/y	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000

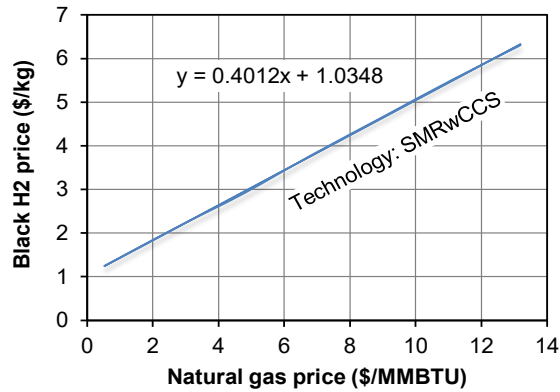
**Table S7.4.** Assumption and estimated techno-economic characteristics for solid oxide electrolyzer cell (SOEC) <sup>58</sup>

	Unit	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Efficiency (LHV)	%	78%	78%	78%	78%	79%	79%	79%	80%	80%	80%	81%
Efficiency	kWh/kgH <sub>2</sub>	43	43	43	42	42	42	42	42	42	42	41
Stack lifetime	Operating hours	20,000	22,000	24,000	26,000	28,000	30,000	32,000	34,000	36,000	38,000	40,000
CAPEX	\$/kW	4,200	3,960	3,720	3,480	3,240	3,000	2,760	2,520	2,280	2,040	1,800
OPEX												
Stack replacement cost	\$/kW	2,100	1,980	1,860	1,740	1,620	1,500	1,380	1,260	1,140	1,020	900
Stack replacement	% of stack	40%	36%	33%	31%	29%	27%	25%	24%	22%	21%	20%
OPEX-FC	% of CAPEX	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%
Capacity	kWh	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000	20,000
Operability	h/y	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000	8,000

**Table S7.5.** Estimated of green hydrogen price in 2020 – 2030

Electrolyzer type	Energy source	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
ALK	SolarPV	5.041	5.068	4.840	4.613	4.388	4.164	3.942	3.722	3.502	3.284	2.924
	Onshore wind	3.589	3.714	3.584	3.454	3.326	3.199	3.073	2.948	2.823	2.700	2.434
	Offshore wind	7.144	7.013	6.627	6.243	5.862	5.483	5.106	4.731	4.358	3.987	3.474
	CSP	10.049	9.815	9.326	8.841	8.358	7.878	7.401	6.926	6.454	5.984	5.372
	Bioenergy	3.890	4.084	4.022	3.962	3.902	3.843	3.784	3.727	3.669	3.613	3.413
	Hydropower	3.138	3.309	3.225	3.141	3.058	2.976	2.895	2.815	2.735	2.656	2.434
	Geothermal	4.390	4.558	4.471	4.384	4.299	4.214	4.130	4.047	3.965	3.883	3.658
PEM	SolarPV	6.532	6.132	5.753	5.392	5.047	4.716	4.397	4.090	3.793	3.505	3.226
	Onshore wind	4.867	4.596	4.343	4.104	3.879	3.664	3.459	3.263	3.075	2.893	2.718
	Offshore wind	8.944	8.339	7.760	7.204	6.668	6.152	5.652	5.168	4.698	4.242	3.798
	CSP	12.274	11.517	10.790	10.090	9.414	8.760	8.127	7.512	6.914	6.334	5.768
	Bioenergy	5.212	5.016	4.835	4.668	4.512	4.365	4.227	4.095	3.970	3.850	3.735
	Hydropower	4.351	4.137	3.940	3.756	3.584	3.422	3.268	3.121	2.981	2.847	2.718
	Geothermal	5.786	5.554	5.339	5.138	4.949	4.770	4.600	4.437	4.282	4.133	3.989
SOEC	SolarPV	10.913	9.922	9.046	8.258	7.540	6.879	6.264	5.687	5.143	4.626	4.133
	Onshore wind	9.667	8.762	7.972	7.269	6.635	6.057	5.525	5.030	4.568	4.132	3.720
	Offshore wind	12.717	11.588	10.575	9.650	8.797	8.001	7.253	6.544	5.868	5.221	4.599
	CSP	15.209	13.988	12.883	11.869	10.925	10.040	9.203	8.406	7.643	6.910	6.202
	Bioenergy	9.924	9.079	8.347	7.702	7.126	6.605	6.129	5.691	5.284	4.904	4.547
	Hydropower	9.280	8.416	7.665	7.001	6.406	5.867	5.374	4.917	4.493	4.095	3.720
	Geothermal	10.354	9.486	8.731	8.063	7.464	6.921	6.423	5.963	5.534	5.133	4.754
ALK	SolarPV&wind-based	4.315	4.391	4.212	4.034	3.857	3.682	3.508	3.335	3.163	2.992	2.679

Also, black H<sub>2</sub> was assumed to be produced via steam methane reforming with carbon capture, in which H<sub>2</sub> price depends on natural gas price, as followed reference <sup>61</sup>, extracted and shown in Fig. S7.1. Noted that future of natural gas price is unstable and not readily available, we estimated based on three big market of natural gas (USA, EU, and Asia) <sup>52,53,62,63</sup>, as shown in Table S7.6.



**Fig. S7.1.** Correlation of H<sub>2</sub> price and natural gas price via technology of steam methane reforming integrated with carbon capture process (SMRwCCS).

**Table S7.6.** Estimation for natural gas prices and black H<sub>2</sub> price

Natural gas price (\$/MMBTU):		2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Market	Assumption													
USA	Pessimistic (World Bank)	3.15	2.50	2.70	2.81	2.92	3.04	3.16	3.29	3.42	3.56	3.70	3.85	4.00
Europe	Medium (World Bank)	7.68	4.50	4.50	4.70	4.92	5.14	5.37	5.61	5.87	6.13	6.41	6.70	7.00
Asia	Optimistic (World Bank)	8.10	8.10	8.11	8.15	8.19	8.23	8.27	8.31	8.35	8.39	8.43	8.47	8.51
USA	Pessimistic (WEO)	3.15	2.66	2.57	2.59	2.61	2.63	2.65	2.67	2.69	2.71	2.73	2.75	2.77
Europe	Medium (WEO)	7.68	4.77	5.96	5.89	5.81	5.74	5.67	5.60	5.53	5.46	5.39	5.33	5.26
Asia	Optimistic (WEO)	8.10	5.73	6.64	6.64	6.65	6.65	6.66	6.67	6.67	6.68	6.68	6.69	6.69
USA	Pessimistic (EIA)	3.15	3.29	3.43	3.58	3.74	3.91	4.08	4.26	4.45	4.64	4.85	5.06	5.28
Europe	Medium (EIA)	7.68	8.02	8.37	8.74	9.12	9.53	9.95	10.38	10.84	11.32	11.82	12.34	12.88
Asia	Optimistic (EIA)	8.10	8.46	8.83	9.22	9.62	10.05	10.49	10.95	11.43	11.94	12.46	13.01	13.58
Black H <sub>2</sub> price (\$/kg):		2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Market	Assumption													
USA	Pessimistic (World Bank)	2.30	2.04	2.12	2.16	2.21	2.25	2.30	2.35	2.41	2.46	2.52	2.58	2.64
Europe	Medium (World Bank)	4.12	2.84	2.84	2.92	3.01	3.10	3.19	3.29	3.39	3.49	3.61	3.72	3.84
Asia	Optimistic (World Bank)	4.28	4.29	4.29	4.30	4.32	4.34	4.35	4.37	4.38	4.40	4.42	4.43	4.45
USA	Pessimistic (WEO)	2.30	2.10	2.07	2.07	2.08	2.09	2.10	2.11	2.11	2.12	2.13	2.14	2.15
Europe	Medium (WEO)	4.12	2.95	3.43	3.40	3.37	3.34	3.31	3.28	3.25	3.23	3.20	3.17	3.15
Asia	Optimistic (WEO)	4.28	3.33	3.70	3.70	3.70	3.70	3.71	3.71	3.71	3.71	3.71	3.72	3.72
USA	Pessimistic (EIA)	2.30	2.35	2.41	2.47	2.54	2.60	2.67	2.74	2.82	2.90	2.98	3.06	3.15
Europe	Medium (EIA)	4.12	4.25	4.39	4.54	4.70	4.86	5.02	5.20	5.38	5.58	5.78	5.98	6.20
Asia	Optimistic (EIA)	4.28	4.43	4.58	4.73	4.90	5.07	5.24	5.43	5.62	5.82	6.03	6.25	6.48

**Table S7.7.** Estimated CO<sub>2</sub>-based fuel UPC in short-term future

	MeOH			FT			DME			Olefin			Gasoline		
	2020	2025	2030	2020	2025	2030	2020	2025	2030	2020	2025	2030	2020	2025	2030
Data	5.96	5.08	3.82	7.32	6.25	4.73	6.41	5.51	4.24	4.82	4.09	3.06	5.98	5.13	3.93
	4.50	4.10	3.33	5.55	5.07	4.00	4.92	4.52	3.74	3.61	3.29	3.00	4.57	4.20	3.45
	8.09	6.41	4.38	9.88	7.86	5.41	8.55	6.86	4.81	6.56	5.18	3.52	8.02	6.41	4.46
	11.03	8.83	6.30	13.43	10.78	7.72	11.52	9.30	6.74	8.97	7.17	5.09	10.83	8.73	6.30
	4.80	4.75	4.32	5.91	5.85	5.33	5.23	5.18	4.74	3.86	3.82	3.47	4.86	4.82	4.40
	4.04	3.88	3.33	5.00	4.80	4.14	4.46	4.30	3.74	3.24	3.11	2.66	4.14	3.98	3.45
	5.31	5.13	4.57	6.52	6.31	5.63	5.74	5.56	4.99	4.28	4.13	3.67	5.35	5.18	4.64
	7.47	5.64	4.13	9.14	6.92	5.10	7.93	6.07	4.55	6.06	4.55	3.31	7.43	5.67	4.22
	5.79	4.57	3.61	7.11	5.64	4.48	6.23	5.00	4.03	4.67	3.68	2.89	5.81	4.65	3.73
	9.91	7.09	4.71	12.08	8.67	5.80	10.39	7.54	5.14	8.05	5.74	3.79	9.76	7.06	4.78

	13.28	9.73	6.70	16.14	11.86	8.20	13.79	10.21	7.15	10.82	7.90	5.42	12.99	9.59	6.69
	6.14	5.28	4.64	7.53	6.49	5.72	6.58	5.72	5.07	4.96	4.26	3.74	6.15	5.33	4.71
	5.27	4.33	3.61	6.47	5.34	4.48	5.70	4.75	4.03	4.25	3.48	2.89	5.31	4.41	3.73
	7.00	5.69	4.90	8.00	6.99	6.03	7.00	6.13	5.33	5.00	4.59	3.95	7.00	5.72	4.96
	11.90	7.82	5.05	14.48	9.56	6.21	12.40	8.28	5.48	9.69	6.34	4.07	11.67	7.76	5.10
	10.64	6.99	4.63	12.96	8.56	5.70	11.13	7.44	5.06	8.65	5.66	3.72	10.46	6.97	4.70
	13.73	8.96	5.52	16.68	10.93	6.78	14.25	9.43	5.95	11.18	7.27	4.45	13.42	8.85	5.55
	16.25	11.02	7.14	19.73	13.42	8.73	16.79	11.51	7.59	13.25	8.96	5.78	15.84	10.83	7.11
	10.90	7.55	5.46	13.28	9.23	6.71	11.39	8.00	5.90	8.87	6.12	4.41	10.71	7.50	5.50
	10.25	6.80	4.63	12.49	8.33	5.70	10.74	7.25	5.06	8.33	5.50	3.72	10.09	6.78	4.70
	11.34	7.87	5.67	13.80	9.61	6.97	11.83	8.33	6.11	9.22	6.38	4.58	11.13	7.80	5.70
Mean	8.74	6.55	4.78	10.64	8.02	5.88	9.19	6.99	5.21	7.06	5.30	3.87	8.64	6.54	4.85

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