Supporting Information

Comparative Life Cycle Assessment of Electrochemical Upgrading of CO_2 to Fuels and Feedstocks

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Thermochemical CO_2 Utilization Process

For thermochemical processes, hydrogen is considered to be supplied by water electrolysis (50 kWh/kg H_2).[1]

Table S1: Thermochemical processes for the CO_2-derived products

Product	System Description	References
Syngas ($CO+H_2$)	**Process 1:** Reverse water-gas shift reaction (rWGS) $CO_2 + H_2 \rightarrow CO + H_2O$, at 200-600°C, 30 bar **Process 2:** Dry reforming of methane (DRM) $CO_2 + CH_4 \rightarrow 2CO + 2 H_2$, at 750°C,	2,3
Formic Acid	**Process 1:** Equimolar hydrogenation: at 140°C, 30 bar $CO_2 + H_2 \rightarrow HCOOH$ **Process 2:** rWGS followed by carbonylation $CO_2 + H_2 \rightarrow CO + H_2O$, : at 650-1100°C, 30 bar $CO \rightarrow HCOOH$	4
Methane	Sabatier reaction: at 280-300°C, 5-8 bar $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$	5,6
Methanol	**Process 1:** CO_2 hydrogenation $CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$, at 210-250°C, 50-75 bar **Process 2:** CO_2-based Syngas route $CO_2 + H_2 \rightarrow CO + H_2O$, at 200-600°C, 30 bar $CO + 2H_2 \rightarrow CH_3OH$	4,7,8
Ethylene	CO_2 hydrogenation: at 400°C, 15 bar $2CO_2 + 6H_2 \rightarrow C_2H_4 + H_2O$	9

Table S2: Incumbent/commercial production processes for the eight products of interest

Product	System Description	References
Syngas ($CO+H_2$)	**Process 1:** Steam-methane-reforming (SMR): at 850-900 °C, 10-30 bar, with nickel as catalyst $CH_4 + H_2O \rightarrow CO + 3H_2$ **Process 2:** Gasification of coal: 600-1900 °C, 80 atm $3C + O_2 + H_2O \rightarrow 3CO + H_2$	[10,11]
Formic Acid	Step 1 – CO production via SMR Step 1 – methanol carbonylation: at 80°C, 45 bar $CH_3OH + CO \rightarrow HCOOCH_3$ Step 2 – hydrolysis of methyl formate $HCOOCH_3 + H_2O \rightarrow CH_3OH + HCOOH$	[12]
Methane	**Process 1:** Natural gas (75-99 vol% methane) as fossil equivalent **Process 2:** Sabatier reaction: at 300-400°C, 5-8 bar, with nickel as catalyst $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$	[13,14]
Methanol	Step 1 – syngas production via SMR Step 2 – syngas conversion: at 200-300 °C, 50-100 bar $CO + 2H_2 \rightarrow CH_3OH$	[15]
Ethylene	Pyrolysis of hydrocarbons: at 600-900°C $C_aH_b \rightarrow C_2H_4 + H_2 + C_xH_y$	[16]
Ethanol	**Process 1:** Fermentation of Corn: $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$ **Process 2:** Hydration of ethylene: at 260-315°C, 55-75 bar, with phosphoric acid (V) as catalyst $C_2H_4 + H_2O \rightarrow C_2H_5OH$	[17,18]
Acetic Acid	Carbonylation of methanol with carbon monoxide: at 190°C, 9 atm, with iridium/ruthenium as catalyst $CH_3OH + CO \rightarrow CH_3COOH$	[19]
n-Propanol	Hydroformylation of ethylene: at 80-150°C, 12-50 bar, with rhodium as catalyst $C_2H_4 + CO + 2H_2 \rightarrow C_3H_7OH$	[20]

Table S3: Gibb's free energy of formation (ΔG^0_f)[21,22]

Component	Molecular Formula	ΔG^0_f (kJ / mol)
Water	H_2O	-237.1
Oxygen	O_2	0
Carbon dioxide	CO_2	-394.4
Carbon monoxide	CO	-137.2
Formic acid	HCOOH	-361.4
Methane	CH_4	-50.5
Methanol	CH_3OH	-166.6
Ethylene	C_2H_4	68.4
Ethanol	C_2H_5OH	-174.8
Acetic acid	CH_3COOH	-389.9
n-Propanol	C_3H_7OH	-171.3

All in standard conditions (1 bar, 298K)

Table S4: Higher heating value of products[23,24]

Products	Higher Hating Value (MJ/kg)
Hydrogen	141.88
Carbon monoxide	10.1
Formic acid	5.52
Methane	55.6
Methanol	22.88
Ethylene	50.3
Ethanol	29.84
Acetic Acid	14.55
n-propanol	33.62

Table S5: PSA separation energy for gaseous products (per kg product)

Products		Single Pass Conversion (%)	CO_2 Conversion (%)[25]	Actual CO_2 Required (kg)	HCO_3^- Formation (%)[25]	HCO_3^- Formation(kg)	Cathodic Gas Volume and PSA Energy									Anodic Gas Volume and PSA Energy						CO_2 to CO Separation (kWh/kg)	Overall PSA Energy (kWh)
							Outlet CO_2/CO (kg)	Outlet CO_2/CO (m_3)	Outlet Product (kg)	Outlet Product (m_3)	Outlet H_2 (kg)	Outlet H_2 (m_3)	Total Volume (m_3)	1st PSA Energy (kWh)	2nd PSA Energy (kWh)	Outlet CO_2/CO (kg)	Outlet CO_2/CO (m_3)	Outlet O_2 (kg)	Outlet O_2 (m_3)	Total Volume (m_3)	3rd PSA Energy (kWh)		
Formic Acid	One-step	50	50	1.91	50	0.96	0.96	0.48	1	-	0.005	0.05	0.54	0.13	-	0.96	0.48	0.35	0.24	0.73	0.18	-	0.32
Syngas (CO+H_2)	One-step	50	100#	3.14	0	-	1.57	1.37	1	0.87	0.008	0.09	2.34	0.59	0.37	-	-	0.57	0.39	0.39	-	-	0.95
Methane	One-step	50	20	13.7	80	10.96	2.74	1.38	1	1.52	0.06	0.62	3.52	0.88	0.50	10.96	5.54	3.99	2.79	8.33	2.08	-	3.46
	Two-step	50	-	2.74	-	-	1.75	1.54	1	1.52	0.04	0.47	3.52	0.88	0.50	-	-	2.99	2.09	2.09	-	1.67	3.05
Methanol	One-step	50	25	5.48	75	4.11	1.37	0.69	1	-	0.02	0.23	0.93	0.23	-	4.11	2.08	1.50	1.05	3.12	0.78	-	1.01
	Two-step	50	-	1.37	-	-	0.874	0.76	1	-	0.01	0.16	0.92	0.23	-	-	-	0.99	0.69	0.69	-	0.83	1.06
Ethylene	One-step	50	25	12.52	75	9.42	3.14	1.59	1	0.85	0.05	0.53	2.97	0.74	0.53	9.42	4.76	3.42	2.39	7.15	1.79	-	3.06
	Two-step	50	-	3.14	-	-	2	1.75	1	0.85	0.03	0.36	2.96	0.74	0.53	-	-	2.28	1.59	1.60	-	1.90	3.17
Ethanol	One-step	50	25	7.64	75	5.73	1.91	0.96	1	-	0.03	0.32	1.29	0.32	-	5.73	2.89	2.08	1.46	4.35	1.09	-	1.41
	Two-step	50	-	1.92	-	-	1.22	1.07	1	-	0.02	0.21	1.28	0.32	-	-	-	1.39	0.97	0.97	-	1.16	1.48
Acetic Acid	One-step	50	33.5	4.45	67.5	2.98	1.47	0.74	1	-	0.01	0.17	0.91	0.23	-	2.98	1.51	1.07	0.75	2.25	0.56	-	0.79
	Two-step	50	-	1.46	-	-	0.93	0.82	1	-	0.01	0.08	0.89	0.22	-	-	-	0.53	0.37	0.37	-	0.89	1.11
n-Propanol	One-step	50	25	8.76	75	6.57	2.19	1.11	1	-	0.03	0.37	1.48	0.37	-	6.57	3.32	2.39	1.68	4.99	1.25	-	1.62
	Two-step	50	-	2.19	-	-	1.4	1.23	1	-	0.02	0.24	1.48	0.37	-	-	-	1.59	1.12	1.12	-	1.33	1.70

*Assumed basis for PSA separation – **0.25 kWh/Nm^3** for all gaseous products[26]

*Density of gases: H_2 = 0.089 kg/m^3, CO = 1.14 kg/m^3, CO_2 = 1.98 kg/m^3, O_2 = 1.429 kg/m^3, CH_4 = 0.657 kg/m^3, C_2H_4 = 1.18 kg/m^3

***Outlet gas = CO_2 (one-step), CO (two-step)

*No HCO_3^- formation has been considered in two-step process

Based on solid-oxide electrolysis cell (SOEC) for $CO_2 \rightarrow CO$ and considering no HCO_3^- formation

Table S6: Energy breakdown for electrochemical conversion (one-step vs two-step)

Products		Capture Energy (kWh/kg)*	Conversion Energy (kWh/kg)	Separation Energy (kWh/kg)	10% BoP (kWh / kg)	Total (kWh/kg)
Formic Acid	One-step	0.34	3.62	22.04	0.36	26.36
	Two-step		-	-	-	-
Syngas ($CO+H_2$)	One-step	0.56	15.11#	0.95	1.51	18.13
	Two-step		-	-	-	-
Methane	One-step	0.97	36.54	3.46	3.65	44.63
	Two-step		25.00	3.04	2.50	31.51
Methanol	One-step	0.48	14.57	27.44	1.46	43.96
	Two-step		10.28	27.49	1.03	39.29
Ethylene	One-step	1.11	32.49	3.06	3.25	39.91
	Two-step		22.69	3.17	2.27	29.24
Ethanol	One-step	0.68	19.74	17.26	1.97	39.65
	Two-step		13.78	17.33	1.38	33.17
Acetic Acid	One-step	0.52	10.04	25.31	1.00	36.87
	Two-step		7.05	25.63	0.71	33.90
n-Propanol	One-step	0.77	22.56	10.22	2.26	35.81
	Two-step		15.70	10.30	1.57	28.35

#CO is commercially available as syngas ($CO+H_2$). Functional unit has been taken as 1 kg CO+0.216 kg H_2 for consistent comparison with incumbent and thermochemical processes.[27] Thus, conversion energy of CO contains energy for 1 kg CO and 0.216 kg H_2 from water electrolysis (50 kWh/kg H_2[28]).

*Capture energy is calculated based on CO_2 requirement per kg product, average capture energy for a power plant (3vol% CO_2) = **0.354 kWh/kg CO_2**[29]

*Assumed basis for PSA separation – **0.25 kWh/Nm^3** for all gaseous products[26]

* 95% energy conversion efficiency (thermal to electrical) for distillation have been assumed.[30]

Table S7: Global warming impact (GWI) for eight electrochemical CO_2 reduction products

CO_2 derived products via one or two step electrochemical conversion routes		Capture emissions* (kg CO_2e/kg product)	Capture emissions# (kg CO_2e/kg product)	Carbon credit for H_2 (kg CO_2e/kg product)	Conversion emissions (kg CO_2e/kg product)	Separation emissions (kg CO_2e/kg product)	Emissions from BOP (kg CO_2e/kg product)	Net GWI* (kg CO_2e/kg product)	Net GWI# (kg CO_2e/kg product)
Formic acid	**One-step**	-0.76	-0.48	-0.04	0.62	3.74	0.06	3.62	3.91
Syngas ($CO+H_2$)	**One-step**	-1.25	-0.78	-0.07	2.57	0.16	0.27	1.66	2.13
Methane	**One-step**	-2.19	-1.37	-0.47	6.21	0.59	0.62	4.76	5.58
	Two-step			-0.35	4.25	0.52	0.43	2.65	3.47
Methanol	**One-step**	-1.09	-0.69	-0.17	2.48	4.66	0.25	6.11	6.53
	Two-step			-0.12	1.75	4.67	0.17	5.38	5.79
Ethylene	**One-step**	-2.51	-1.57	-0.40	5.52	0.52	0.55	3.68	4.63
	Two-step			-0.27	3.86	0.53	0.39	2.00	2.94
Ethanol	**One-step**	-1.53	-0.96	-0.25	3.36	2.93	0.34	4.85	5.42
	Two-step			-0.16	2.34	2.95	0.23	3.84	4.41
Acetic acid	**One-step**	-1.18	-0.74	-0.13	1.71	4.30	0.17	4.87	5.31
	Two-step			-0.06	1.19	4.36	0.12	4.44	4.88
n-Propanol	**One-step**	-1.75	-1.1	-0.28	3.84	1.74	0.38	3.92	4.58
	Two-step			-0.19	2.67	1.75	0.27	2.75	3.40

EEF = 0.17 kg CO_2e/kWh (see details in Table S6)

*Assumed footprint for carbon feedstock is -0.8 kg CO_2e/kg CO_2 capture[31]

Assumed footprint for carbon feedstock is -0.5 kg CO_2e/kg CO_2 capture[31]

<u>Renewable Energy Utilization (Perspective of Canada)</u>[32]

Electricity emission factor, EEF has been taken as **0.17 kg CO_2e/kWh** (representing average carbon intensity for present-day electricity generation in Canada).

Table S8: EEF based on percentage calculation for renewable share for Canadian electricity generation[32]

Renewable Share	**EEF (kg CO_2e/kWh)**
50%	0.17
66%	0.12
80%	0.07
90%	0.035

GWI of O_2, H_2 and H_2O (One-step Methanol as Reference)

a) **For O_2:**[33]

Based on cryogenic super critical air separation,

Specific energy demand for O_2 supply = 200 kWh/tonne O_2

Overall CO_2 emission = $0.17\frac{kg}{kWh} * 200\frac{kWh}{t\,O_2} * \frac{1\,t}{1000\,kg}$ = **0.034 kg/kg O_2**

For methanol, 1.66 kg O_2 is produced per kg methanol.

Thus, environmental burden from O_2 production = $\frac{0.034\,kg\,CO_2e}{kg\,O_2} * \frac{1.66\,kg\,O_2}{kg\,methanol} =$ **0.06 kg CO_2e/kg methanol**

b) **For H_2:**[1]

H_2 supply has been considered by polymer electrolyte membrane-based water electrolysis.

GWI of H_2 via water electrolysis = $0.17\frac{kg}{kWh} * 50\frac{kWh}{kg\,H_2}$ = **8.50 kg CO_2e/kg H_2**

For methanol, 0.02 kg H_2 is produced (10% selectivity) per kg methanol.

Thus, environmental burden from H_2 production = $\frac{8.5\,kg\,CO_2e}{kg\,H_2} * \frac{0.02\,kg\,H_2}{kg\,methanol} =$ **0.17 kg CO_2e/kg methanol**

c) **For H_2O:**[34]

Underground water pumping energy = 0.45 kWh/m^3

Average treatment energy before supply = 0.327 kWh/m^3

Total energy = 0.78 kWh/m^3 = (0.78/1000) = $\frac{0.78\,kWh}{m^3} * \frac{m^3}{1000\,kg}$ = 7.8×10^{-4} kWh/kg

EEF = 0.17 kg CO_2e/kWh

GWI for water treatment and supply = $\frac{0.00078\,kWh}{kg} * \frac{0.17\,kg\,CO_2e}{kWh}$ = **1.326×10^{-4} kg CO_2e/kg H_2O**

For methanol, 0.94 kg water is required per kg methanol.

Thus, GWI = $\frac{0.000133\,kg\,CO_2e}{kg\,H_2O} * \frac{0.94\,kg\,H_2O}{kg\,methanol} =$ **0.00012 kg CO_2e/kg methanol**

Table S9: Comparison between electrochemical and thermochemical CO_2 conversion as compared to incumbent routes

	Incumbent		Electrochemical CO_2 conversion (with -0.8 kg CO_2e/kg CO_2 as capture footprint)		Thermochemical CO_2 conversion
Products	**Industrial Production Process**	**GWI (kg CO_2e/kg)**	**One-step, GWI (kg CO_2e/kg)**	**Two-step GWI (kg CO_2e/kg)**	**GWI (kg CO_2e/kg)#**
Formic acid	Methyl formate hydrolysis	1.1-1.5[27]	3.62	-	0.54-1.58[27]
Syngas ($CO+ H_2$)	- Steam-methane-reforming - Coal gasification	1.74[27]	1.66	-	1.92-2.51[27]
Methanol	Reforming of syngas	0.68-1.08[27]	6.11	5.38	1.21-1.44[27]
Methane	- Natural gas (75-99 vol% methane) - Sabatier reaction	0.66[28] 0.46[35] 0.5[27]	4.76	2.65	3.0-5.0[27]
Ethylene	Steam cracking of naptha	1.9[36,77]	3.68	2.00	3.30[37]
Ethanol	- Corn fermentation - Ethylene hydration	0.00[38] -0.5[39,40]	4.85	3.84	N/A
Acetic Acid	Methanol carbonylation with CO	1.75[36]	4.87	4.44	N/A
n-Propanol	Hydroformylation of ethylene	4.44***	3.92	2.75	N/A

*EEF = 0.17 kg CO_2e/kWh (see details in Table S6)

***ecoinvent V3.5 (IPCC GWP100a), #We assumed similar environmental impact (GWI) of steam-methane-reforming and water electrolysis for H_2 supply at 0.17 kg CO_2e/kWh.

Calculation for EE (with One-step Methanol as Reference)

Assuming 1000 kg/day basis of methanol,

Calculated thermodynamic voltage = 1.21 V

Assumed anodic overpotential = 0.8 V

Assumed cathodic overpotential = 0.6 V

Total voltage = 1.21 + 0.6 + 0.8 V = 2.61 V

Assumed faradaic efficiency = 90%

Number of electrons per mole = 6

Molar mass = 32.04

Calculated current = $\frac{1000\ kg\ \ 1\ day\ \ 1000\ g\ \ \ mol}{day\ \ \ 86400\ s\ \ 1\ kg\ \ 32.04\ g} * 6e^{-} * \frac{96485\ C}{mol} =$ 209124.45 A = 209.12 A/kg

Total current = $\frac{209.12\ A}{0.9}$ = 232.36 A

Electrochemical conversion energy = $232.36\ A * 2.61\ V * 24h * \frac{1\ kWh}{1000\ Wh} = 14.55\ kWh$

Higher heating value = $22.88\ MJ * \frac{.277\ kWh}{1\ MJ} = 6.36\ kWh$

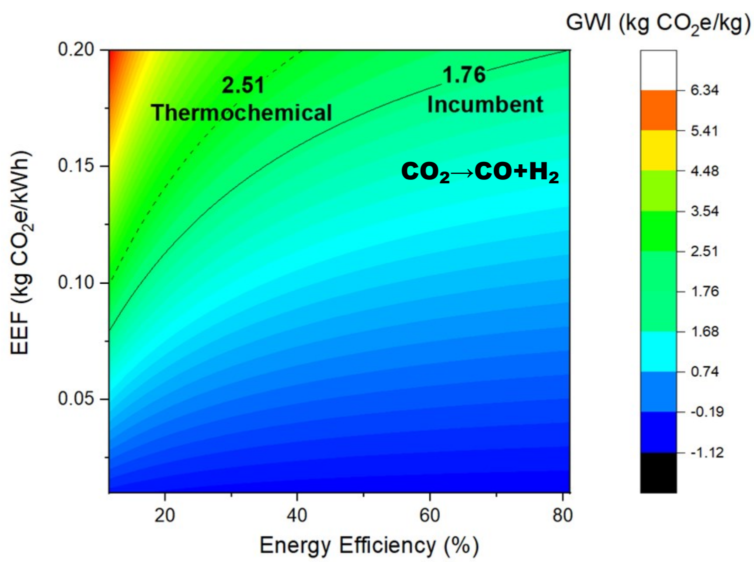
Thus, energy efficiency = $\frac{6.36\ kWh}{14.55\ kWh} = 43.7\%$

Table S10: Future projections for electricity emission factor (EEF) for US grid mix[41]

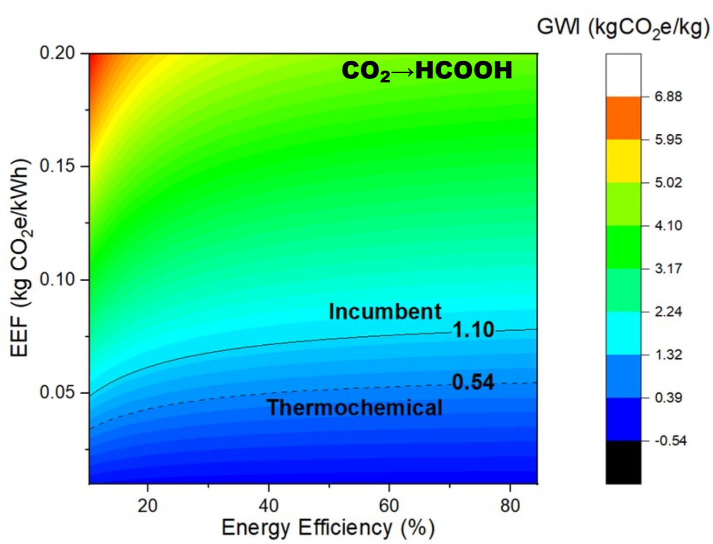
Year	Projected Renewable Share (%)	Projected EEF (kg CO_2e/kWh)
2020	20	0.430
2030	33	0.317
2040	41	0.297
2050	51	0.256

Contour Plots for Electrochemical CO_2- Derived Products

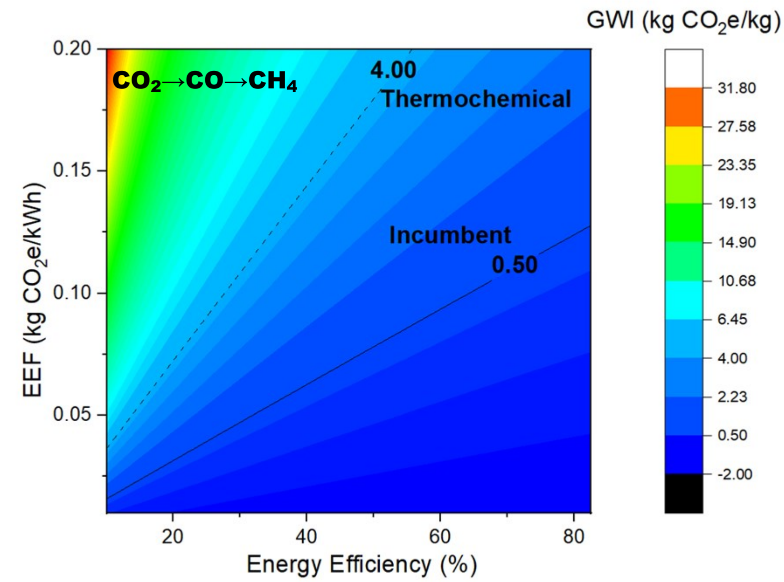
a)



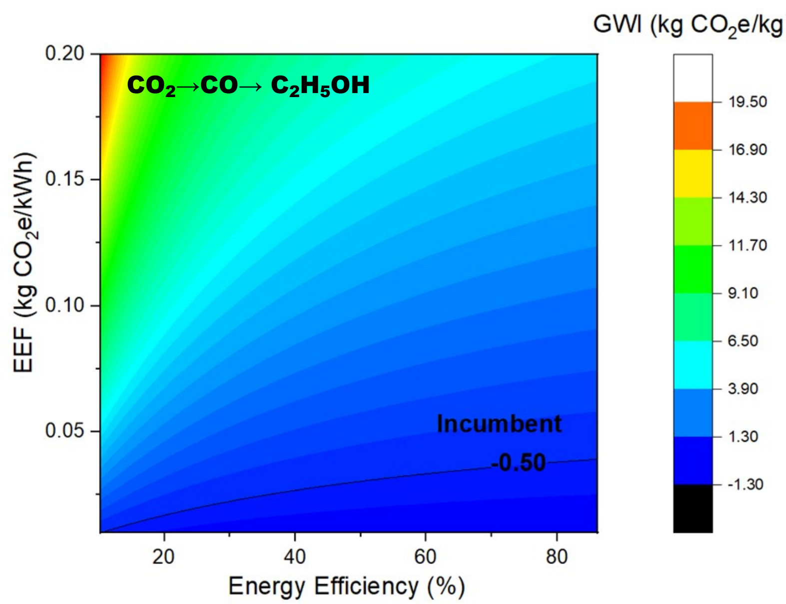
b)



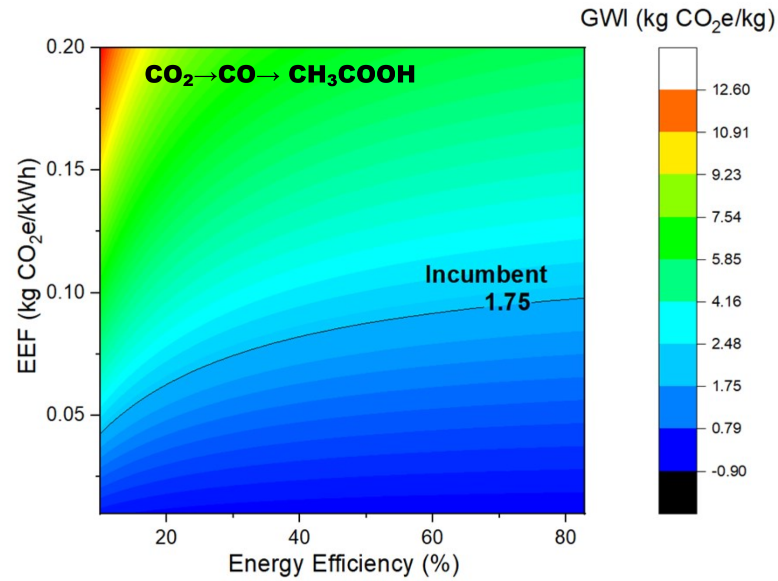
c)


GWI (kg CO_2e/kg)
CO_2→CO→CH_4
4.00
Thermochemical
Incumbent
0.50
EEF (kg CO_2e/kWh)
Energy Efficiency (%)
31.80
27.58
23.35
19.13
14.90
10.68
6.45
4.00
2.23
0.50
-2.00

d)


GWI (kg CO_2e/kg)
CO_2→CO→ C_2H_5OH
Incumbent
-0.50
EEF (kg CO_2e/kWh)
Energy Efficiency (%)
19.50
16.90
14.30
11.70
9.10
6.50
3.90
1.30
-1.30

e)



f)

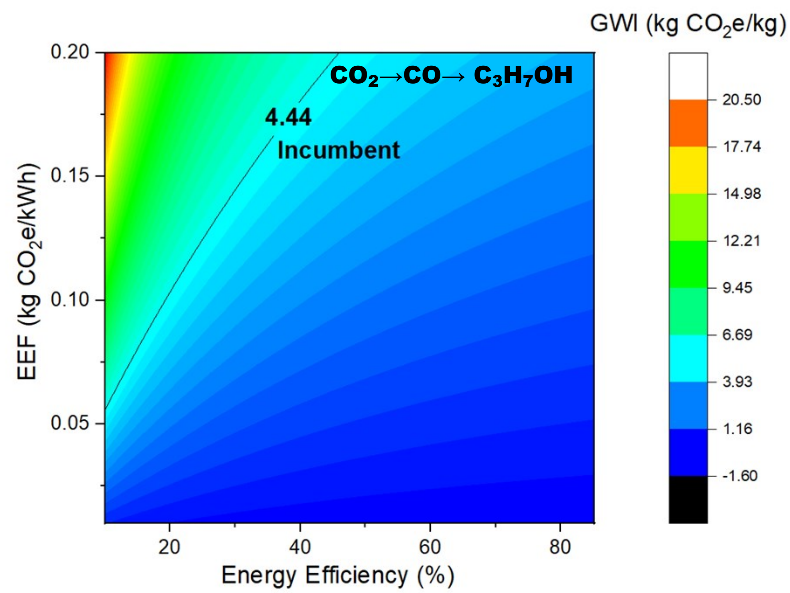


Figure S1: Effect of EEF and EE on GWI for electrosynthesis products. a) Syngas, b) Formic acid, c) Methane, d) Ethanol, e) Acetic acid, f) n-Propanol. 10wt% feed concentration has been considered for liquid products. CO_2 capture footprint has been considered as -0.8 kg CO_2e/kg CO_2 captured.

<u>Relation Between Distillation Feed Concentration with Energy for Separation</u>

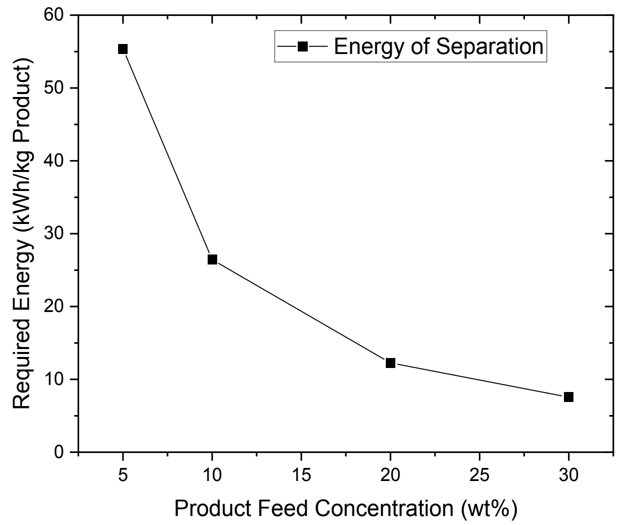


Figure S2: Relation between feed concentration in distillation and required energy for separation (with methanol as reference)

Sensitivity Analysis for Electrosynthesis of Two-step Methanol

Table S11: Performance metrics for sensitivity analysis

	Scenario 1	Base case	Scenario 2
Faradaic Efficiency (%)	45	90	100
Overpotential (V)	0.3	0.6	0.9
PSA Energy (kWh/kg)	0.125	0.25	0.375
CO_2 Capture Footprint (kg CO_2e/kg CO_2)	-0.4	-0.8	-1.2
Product Feed Concentration (wt%)	5	10	15

*EEF = 0.17 kg CO_2e/kWh

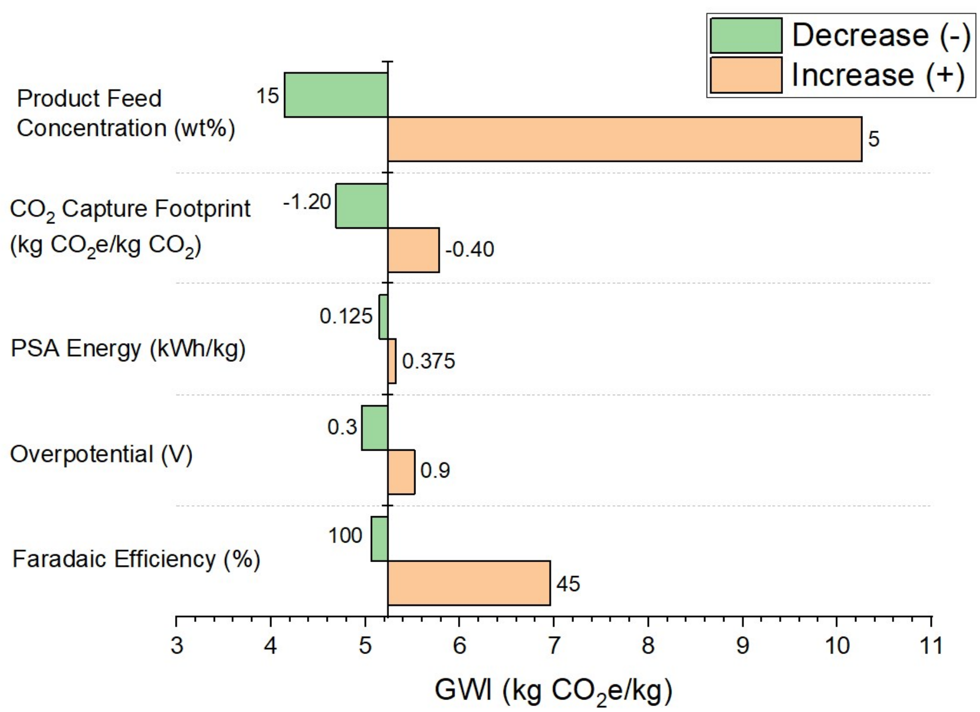


Figure S3: Sensitivity analysis for two-step methanol based on performance metrics

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