Electronic Supplementary Information

Catholyte-free electroreduction of CO_2 for sustainable production of CO: Concept, process development, technoeconomic analysis, and CO_2 reduction assessment

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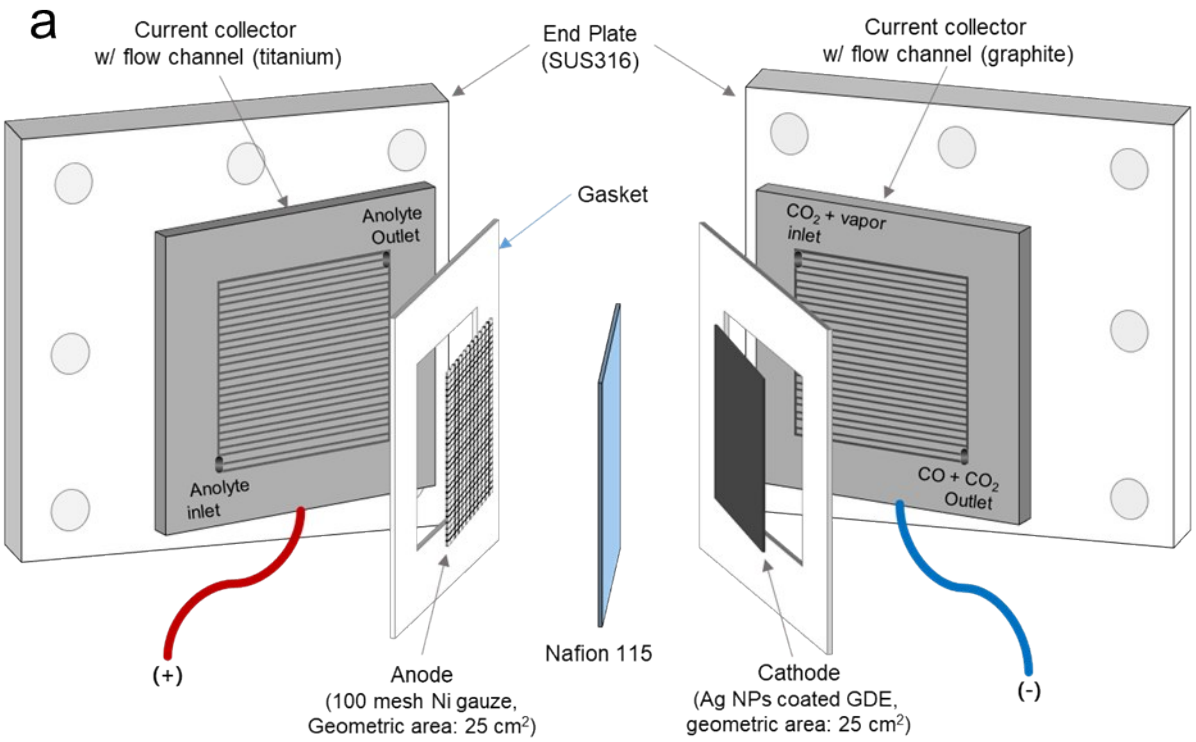

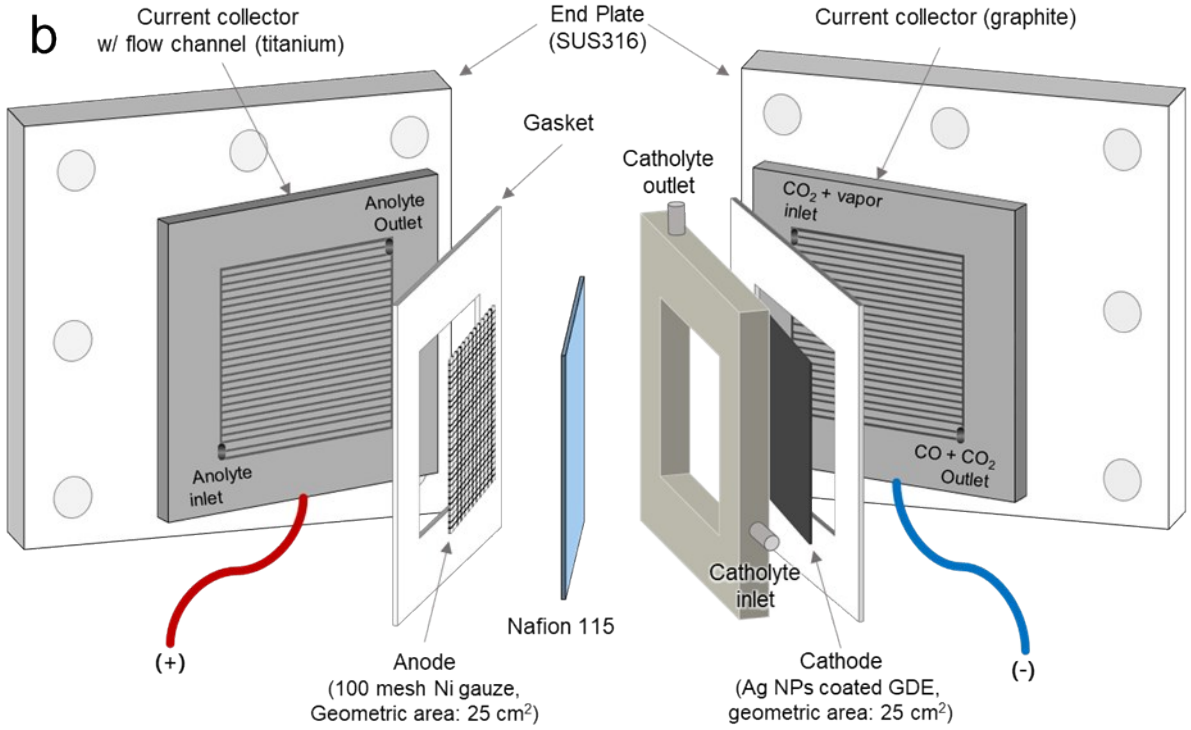

1. Construction of full flow cells for the CF-ECO2R and GDE-catholyte systems

Fig. S1. Construction of a full flow cell for a) the CF-ECO_2R and b) GDE-catholyte systems.

2. Combination of 3-stage membrane and oxy-combustion process (Case 1)

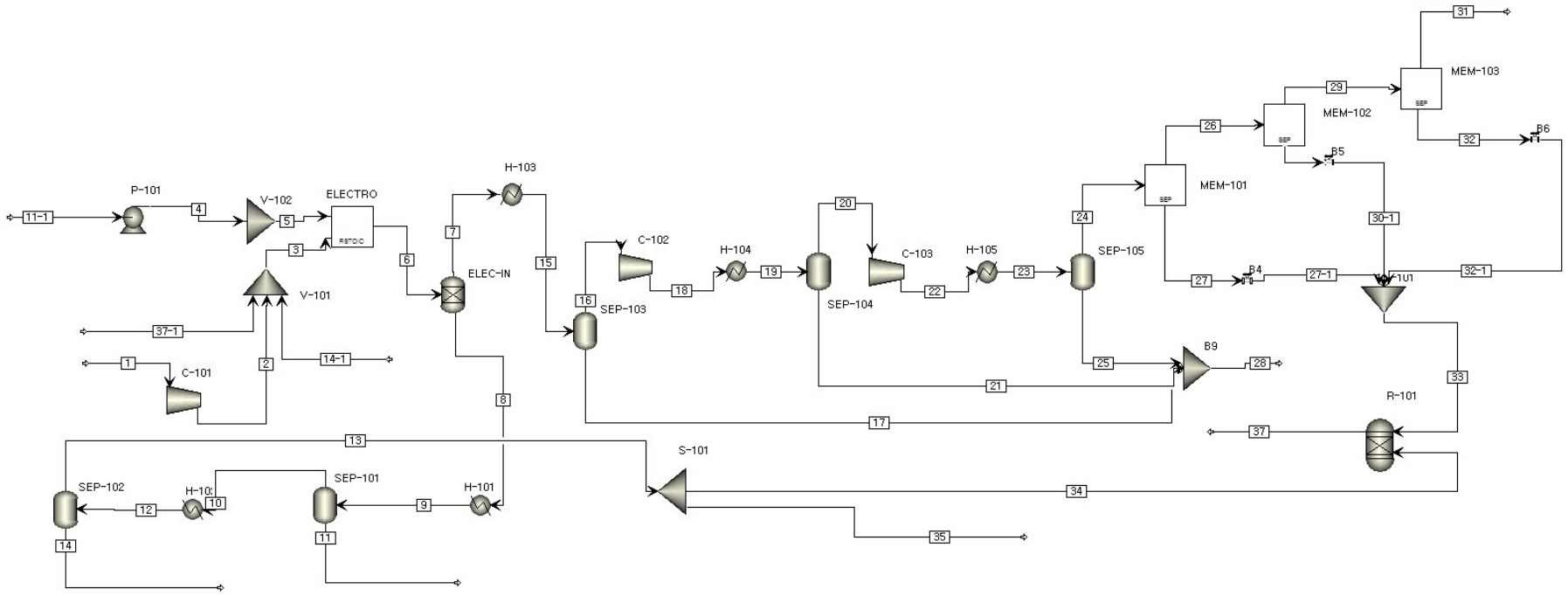

Fig. S2. PFD of Case 1: combination of 3-stage membrane and oxy-combustion process.

Table S1. Stream table (Case 1)

	Units	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Temperature	C	100	126.7	89	89	89	40	40	40	90	90
Pressure	bar	1	1.28	1	1.5	1	1	1	1	1	1
Mass flow rate	kg/hr	140,368	140,368	168,464	3,645,763	3,645,763	3,814,227	118,840	3,695,387	3,695,387	63,172
Mole flow rate	kmol/hr	3,282	3,282	4,841	202,370	202,370	208,108	3,679	204,430	204,430	2,846
Volume flow rate	L/sec	28,280	23,676	45,041	1,089	1,089	44,093	29,156	10,009	24,953	23,867
Mass flow rate											
H_2O	kg/hr	2,807	2,807	30,904	3,645,763	3,645,763	3,675,650	8,951	3,666,699	3,666,699	35,925
CO	kg/hr	0	0	0	0	0	48,645	48,645	0	0	0
CO_2	kg/hr	137,561	137,561	137,561	0	0	61,131	61,131	0	0	0
H_2	kg/hr	0	0	0	0	0	114	114	0	0	0
O_2	kg/hr	0	0	0	0	0	28,688	0	28,688	28,688	27,248
	Units	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Temperature	C	90	30	30	30	40	40	40	149.1	25	25
Pressure	bar	1	1	1	1	1	1	1	2.5	2.5	2.5
Mass flow rate	kg/hr	3,632,215	63,172	27,853	35,319	118,840	114,382	4,458	114,382	114,382	110,390
Mole flow rate	kmol/hr	201,583	2,846	887	1,959	3,679	3,433	245,781	3,433	3,433	3,217
Volume flow rate	L/sec	1,086	6,219	6,209	10	29,156	24,830	1	13,392	8,862	8,861
Mass flow rate											
H_2O	kg/hr	3,630,775	35,925	678	35,247	8,951	4,546	4,406	4,546	4,546	722
CO	kg/hr	0	0	0	0	48,645	48,641	3	48,641	48,641	48,632
CO_2	kg/hr	0	0	0	0	61,131	61,082	49	61,082	61,082	60,923
H_2	kg/hr	0	0	0	0	114	114	0	114	114	114
O_2	kg/hr	1,440	27,248	27,125	72	0	0	0	0	0	0
	Units	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**27-1**	**28**	**29**
Temperature	C	25	161.4	25	25	25	25	25	25	31.7	25
Pressure	bar	2.5	8	8	8	8	8	8	1	1	8
Mass flow rate	kg/hr	3,992	110,390	110,390	109,808	582	47,822	61,986	61,986	9,032	32,301
Mole flow rate	kmol/hr	216	3,217	3,217	3,187	30	1,595	1,592	1,592	492	1,136

Volume flow rate	L/sec	1	4,036	2,743	2,743	0	1,373	1,364	10,779	17	978
Mass flow rate											
H_2O	kg/hr	3,824	722	722	214	507	0	214	214	8,737	0
CO	kg/hr	9	48,632	48,632	48,628	4	38,805	9,823	9,823	16	30,967
CO_2	kg/hr	159	60,923	60,923	60,852	71	9,006	51,846	51,846	279	1,333
H_2	kg/hr	0	114	114	114	Trace	11	103	103	0	1
O_2	kg/hr	0	0	0	0	0	0	0	0	0	0
	Units	**30**	**30-1**	**31**	**32**	**32-1**	**33**	**34**	**35**	**37**	
Temperature	C	25	25	2	25	25	21.5	30	30	25	
Pressure	bar	8	1	8	8	1	1	1	1	1	
Mass flow rate	kg/hr	15,522	15,522	24,909	7,392	7,392	84,899	14,926	12,927	99,825	
Mole flow rate	kmol/hr	459	459	887	250	250	2,300	475	412	2,320	
Volume flow rate	L/sec	395	3,161	763	215	1,719	15,652	3,328	2,882	15,978	
Mass flow rate											
H_2O	kg/hr	0	0	0	0	0	214	363	315	1,593	
CO	kg/hr	7,839	7,839	24,711	6,255	6,255	23,917	0	0	0	
CO_2	kg/hr	7,673	7,673	197	1,136	1,136	60,654	0	0	98,232	
H_2	kg/hr	10	10	0	1	1	114	0	0	0	
O_2	kg/hr	0	0	0	0	0	0	14,563	12,613	0	

3. Combination of 3-stage membrane and amine-based CO_2 absorption process (Case 2)

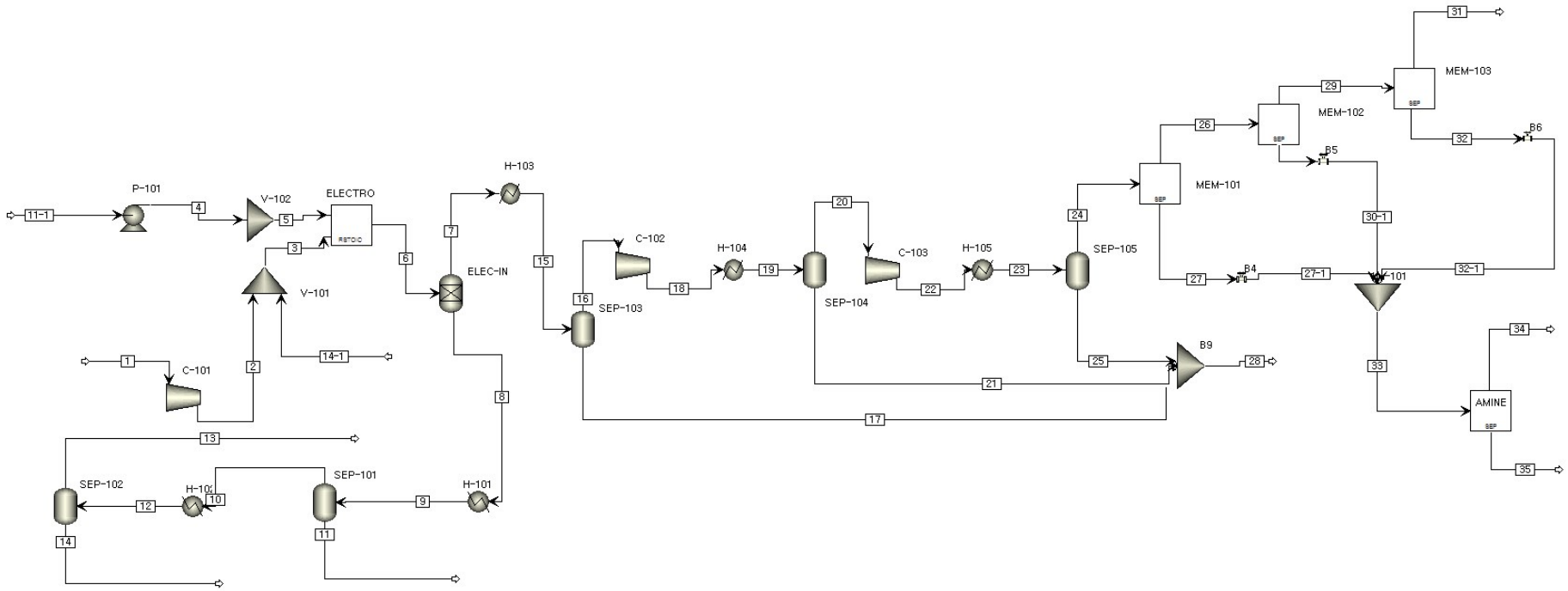

Fig. S3. Detailed system configuration of Case 2: combination of 3-stage membrane and amine-based CO_2 absorption process.

Table S2. Stream table (Case 2)

	Units	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Temperature	C	100	126.7	89	89	89	40	40	40	90	90
Pressure	bar	1	1.28	1	1.5	1	1	1	1	1	1
Mass flow rate	kg/hr	140,368	140,368	168,464	3,645,763	3,645,763	3,814,227	118,840	3,695,387	3,695,387	63,172
Mole flow rate	kmol/hr	3,282	3,282	4,841	202,370	202,370	208,108	3,679	204,430	204,430	2,846
Volume flow rate	L/sec	28,280	23,676	45,041	1,089	1,089	44,093	29,156	10,009	24,953	23,867
Mass flow rate											
H_2O	kg/hr	2,807	2,807	30,904	3,645,763	3,645,763	3,675,650	8,951	3,666,699	3,666,699	35,925
CO	kg/hr	0	0	0	0	0	48,645	48,645	0	0	0
CO_2	kg/hr	137,561	137,561	137,561	0	0	61,131	61,131	0	0	0
H_2	kg/hr	0	0	0	0	0	114	114	0	0	0
O_2	kg/hr	0	0	0	0	0	28,688	0	28,688	28,688	27,248
	Units	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Temperature	C	90	30	30	30	40	40	40	149.1	25	25
Pressure	bar	1	1	1	1	1	1	1	2.5	2.5	2.5
Mass flow rate	kg/hr	3,632,215	63,172	27,853	35,319	118,840	114,382	4,458	114,382	114,382	110,390
Mole flow rate	kmol/hr	201,583	2,846	887	1,959	3,679	3,433	245,781	3,433	3,433	3,217
Volume flow rate	L/sec	1,086	6,219	6,209	10	29,156	24,830	1	13,392	8,862	8,861
Mass flow rate											
H_2O	kg/hr	3,630,775	35,925	678	35,247	8,951	4,546	4,406	4,546	4,546	722
CO	kg/hr	0	0	0	0	48,645	48,641	3	48,641	48,641	48,632
CO_2	kg/hr	0	0	0	0	61,131	61,082	49	61,082	61,082	60,923
H_2	kg/hr	0	0	0	0	114	114	0	114	114	114
O_2	kg/hr	1,440	27,248	27,125	72	0	0	0	0	0	0
	Units	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**27-1**	**28**	**29**
Temperature	C	25	161.4	25	25	25	25	25	25	31.7	25
Pressure	bar	2.5	8	8	8	8	8	8	1	1	8
Mass flow rate	kg/hr	3,992	110,390	110,390	109,808	582	47,822	61,986	61,986	9,032	32,301
Mole flow rate	kmol/hr	216	3,217	3,217	3,187	30	1,595	1,592	1,592	492	1,136

Volume flow rate	L/sec	1	4,036	2,743	2,743	0	1,373	1,364	10,779	17	978
Mass flow rate											
H_2O	kg/hr	3,824	722	722	214	507	0	214	214	8,737	0
CO	kg/hr	9	48,632	48,632	48,628	4	38,805	9,823	9,823	16	30,967
CO_2	kg/hr	159	60,923	60,923	60,852	71	9,006	51,846	51,846	279	1,333
H_2	kg/hr	0	114	114	114	Trace	11	103	103	0	1
O_2	kg/hr	0	0	0	0	0	0	0	0	0	0
	Units	**30**	**30-1**	**31**	**32**	**32-1**	**33**	**34**	**35**		
Temperature	C	25	25	2	25	25	21.5	40	60		
Pressure	bar	8	1	8	8	1	1	2	1		
Mass flow rate	kg/hr	15,522	15,522	24,909	7,392	7,392	84,899	60,059	24,840		
Mole flow rate	kmol/hr	459	459	887	250	250	2,300	1,365	935		
Volume flow rate	L/sec	395	3,161	763	215	1,719	15,652	4,936	7,196		
Mass flow rate											
H_2O	kg/hr	0	0	0	0	0	214	11	203		
CO	kg/hr	7,839	7,839	24,711	6,255	6,255	23,917	0	23,917		
CO_2	kg/hr	7,673	7,673	197	1,136	1,136	60,654	60,048	607		
H_2	kg/hr	10	10	0	1	1	114	0	114		
O_2	kg/hr	0	0	0	0	0	0	0	0		

4. Combination of amine-based CO_2 absorption process and H_2 PSA processes (Case 3)

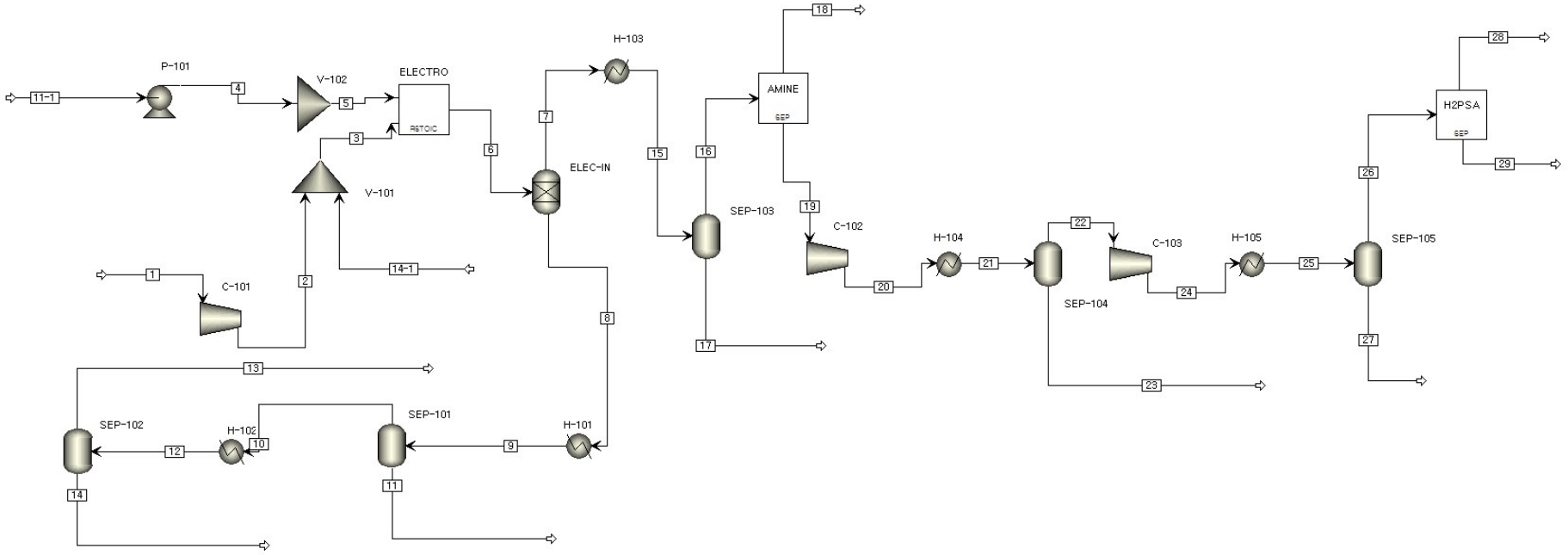

Fig. S4. Detailed system configuration of Case 3: combination of amine-based CO_2 absorption process and H_2 pressure swing adsorption.

Table S3. Stream table (Case 3)

	Units	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Temperature	C	100	126.7	89	89	89	40	40	40	90	90
Pressure	bar	1	1.28	1	1.5	1	1	1	1	1	1
Mass flow rate	kg/hr	71,545	71,545	85,866	1,858,230	1,858,230	1,944,095	60,572	1,883,523	1,883,523	32,199
Mole flow rate	kmol/hr	1,673	1,673	2,468	103,147	103,147	106,072	1,875	104,197	104,197	1,450
Volume flow rate	L/sec	14,414	12,068	22,957	555	555	14,091	12,656	3,273	12,718	12,165
Mass flow rate	kg/hr										
H_2O	kg/hr	1,431	1,431	15,752	1,858,230	1,858,230	1,873,463	4,562	1,868,901	1,868,901	18,311
CO	kg/hr	0	0	0	0	0	24,794	24,794	0	0	0
CO_2	kg/hr	70,114	70,114	70,114	0	0	31,158	31,158	0	0	0
H_2	kg/hr	0	0	0	0	0	58	58	0	0	0
O_2	kg/hr	0	0	0	0	0	14,622	0	14,622	14,622	13,888
	Units	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Temperature	C	90	30	30	30	40	40	40	40	60	194
Pressure	bar	1	1	1	1	1	1	1	2	1	2.5
Mass flow rate	kg/hr	1,851,324	32,199	14,197	18,002	60,572	58,300	2,272	31,108	27,192	27,192
Mole flow rate	kmol/hr	102,746	1,450	452	998	1,875	1,750	125	707	1,043	1,043
Volume flow rate	L/sec	554	3,170	3,165	5	12,656	12,656	1	2,557	8,024	4,5014
Mass flow rate											
H_2O	kg/hr	1,850,590	18,311	346	17,965	4,562	2,317	2,246	6	2,311	2,311
CO	kg/hr	0	0	0	0	24,794	24,792	2	0	24,792	24,792
CO_2	kg/hr	0	0	0	0	31,158	31,133	25	31,102	31	31
H_2	kg/hr	0	0	0	0	58	58	0	0	58	58
O_2	kg/hr	734	13,888	13,851	37	0	0	0	0	0	0
	Units	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	
Temperature	C	25	25	25	141.8	25	25	25	25	25	
Pressure	bar	2.5	2.5	2.5	6	6	6	6	6	6	
Mass flow rate	kg/hr	27,192	25,084	2,109	25,084	25,084	24,958	125	49	24,909	
Mole flow rate	kmol/hr	1,043	926	117	926	926	919	7	24	895	

Volume flow rate	L/sec	2,551	2,550	1	1,479	1,055	1,055	0	28	1,027
Mass flow rate										
H_2O	kg/hr	2,311	211	2,100	211	211	87	124	0	87
CO	kg/hr	24,792	24,784	9	24,784	24,784	24,782	1	0	24,782
CO_2	kg/hr	31	31	0	31	31	31	0	0	31
H_2	kg/hr	58	58	0	58	58	58	0	49	9
O_2	kg/hr	0	0	0	0	0	0	0	0	0

5. Mathematical model for the CF-ECO$_2$R process

Mathematical model for the CF-ECO$_2$R process is referred form published studies.[1-3] The modeling assumptions are summarized as follows:[3, 4]

1. Molar transport phenomena are dominant in the length direction, whereas they are negligible in the directions of cell width and height. Therefore, the model is developed in one dimension to reduce the computational time.
2. Isothermal conditions as validated in the experiments, due to the excess of CO_2 gas and the small cell dimensions.
3. The kinetic rates of the electrochemical reactions can be described by the Butler-Volmer equation, which has been widely used to describe the kinetics of electrochemical reactions.
4. The catalyst layer is treated as an infinitely thin film interface in contact with the electrolyte.
5. Mass transfer limitation is assumed not to play significant role at the current density. The catholyte solution is saturated with CO_2.

The species transport equations are mathematically described by the Nernst-Planck equation.[3, 4]

$$\nabla \cdot N_i = R_i \qquad \text{* MERGEFORMAT (1)}$$

$$N_i = -D_i \nabla C_i - z_i u_{mi} F C_i \nabla \Phi + u C_i \qquad \text{* MERGEFORMAT (2)}$$

$$u_{mi} = \frac{D_i}{RT} \qquad \text{* MERGEFORMAT (3)}$$

where N_i is the species molar flux ($molm^{-2}s^{-1}$); R_i is the reaction rate term of species i; D_i is the diffusion coefficient of species i (m^2s^{-1}); C_i is the molar concentration of species i ($mol \cdot m^{-3}$); z_i is the species charge of species i; u_{mi} is the species mobility of species i ($mol \cdot m^2 \cdot s^{-1} \cdot V^{-1} \cdot C^{-1}$); F is the Faradaic constant ($96,485 Cmol^{-1}$); Φ is the cell potential (V); u is the velocity ($m \cdot s^{-1}$).

The electric potential equation is described as follows:[2-4]

$$\sigma \nabla^2 \Phi = S_\Phi \qquad \text{* MERGEFORMAT (4)}$$

$$S_\Phi = \frac{A_{cell}}{V_{cell}} \sum j_i \qquad \text{* MERGEFORMAT (5)}$$

where σ is the electric conductivity (Sm^{-1}); S_Φ is the sink term in the charge equation; A_{cell} is the area of the computational cell (m^2); V_{cell} is the volume of the computational cell (m^3); j_i is the current density for species i ($A \cdot m^{-2}$).

The reaction kinetics is described by the Butler-Volmer equation.[1-4]

$$j_i = j_{0,i} \left\{ \frac{C_O^{surface}}{C_O^{bulk}} \exp\left[\frac{\alpha_{an,i} nF\eta_i}{RT} \right] - \frac{C_R^{surface}}{C_R^{bulk}} \exp\left[-\frac{\alpha_{ca,i} nF\eta_i}{RT} \right] \right\}$$

* MERGEFORMAT (6)

where j_i is the electrode current density of reaction i ($mAcm^{-2}$); $j_{0,i}$ is the exchange current density of reaction i ($mAcm^{-2}$); $C_O^{surface}$ and $C_R^{surface}$ are the electrode's surface concentration

of the species to be oxidized and to be reduced, respectively; C_O^{bulk} and C_R^{bulk} are the bulk concentration of the species to be oxidized and to be reduced, respectively; n is the electron transfer number of the rate-determining step; $\alpha_{an,i}$ and $\alpha_{ca,i}$ are the anodic and cathodic charge transfer coefficient of reaction i, respectively; R is the universal gas constant ($=8.314 JK^{-1}mol^{-1}$); F is the Faraday constant ($=96485 Cmol^{-1}$); T is the temperature (K); η_i is the electrode overpotential of reaction i (V).

The reaction rate R_i is described as follows:

$$r_{ij} = \frac{\nu_{ij} j_i}{z_j F} \qquad \text{* MERGEFORMAT (7)}$$

$$R_j = \sum_i r_{ij} \qquad \text{* MERGEFORMAT (8)}$$

where r_{ij} is the reaction of species j in reaction i; ν_{ij} is the stoichiometry of species j in the electrochemical reaction i.

Table S4 Estimated values of key model parameters of the CF-ECO$_2$R process

Notation	Estimated value	Unit
α_{rxn3}	0.10	V
α_{rxn4}	0.09	V
$j_{0,rxn3}$	85.6	mAcm^{-2}
$j_{0,rxn4}$	0.20	mAcm^{-2}

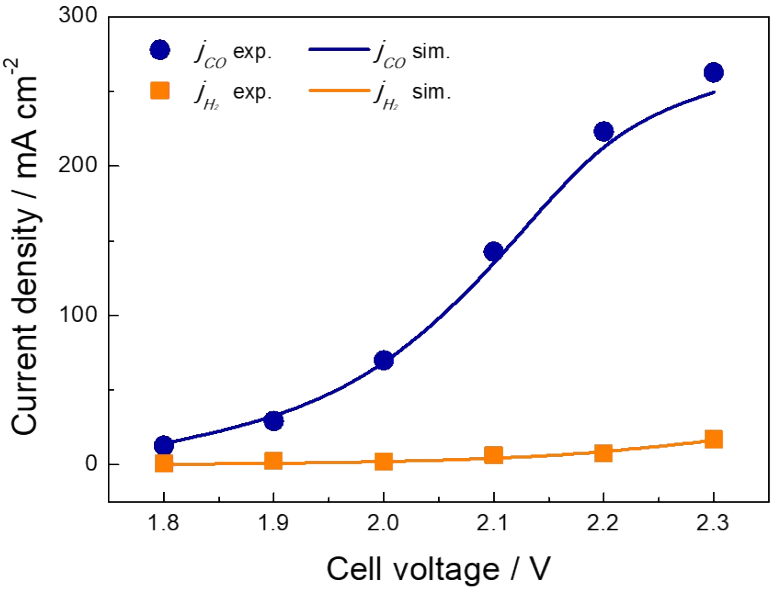

Fig. S5. Verification of the CF-ECO_2R model against experimental data.

6. CO_2 lifecycle assessment method

Lifecycle assessment (LCA) is a method to evaluate and analyze the environmental influences of products and processes taking into consideration their system boundaries and set functional unit. The CO_2 LCA is described by estimating the direct and indirect CO_2 emission and net CO_2 emission, which is calculated by the direct and indirect CO_2 emission.[5-7]

$$F_{CO_2}^{D/I} = F_i \cdot GWP_i \qquad \text{* MERGEFORMAT (9)}$$

$$E_{CO_2}^{D} = \sum \frac{F_{CO_2}^{D}}{F_P} \qquad \text{* MERGEFORMAT (10)}$$

$$E_{CO_2}^{I} = \sum \frac{F_{CO_2}^{I}}{F_P} \qquad \text{* MERGEFORMAT (11)}$$

$$E_{CO_2}^{C} = \sum \frac{F_{CO_2}^{C}}{F_P} \qquad \text{* MERGEFORMAT (12)}$$

$$E_{CO_2}^{N} = E_{CO_2}^{D} + E_{CO_2}^{I} - E_{CO_2}^{C} \qquad \text{* MERGEFORMAT (13)}$$

where F_i is the value of component i (e.g., raw material consumption, utility consumption, etc.) per the set function unit; GWP_i is the life cycle inventory parameter of component i; $E_{CO_2}^{D/I}$ is the direct/indirect CO_2 emission index; $F_{CO_2}^{D/I}$ is the direct/indirect CO_2 emission rate; F_P is the production rate; $E_{CO_2}^{C}$ is the CO_2 consumption index; $F_{CO_2}^{C}$ is the CO_2 consumption rate; $E_{CO_2}^{N}$ is the net CO_2 emission index. Using the $E_{CO_2}^{N}$ value, the CO_2 emission effect of the CO_2 utilization process is evaluated.

The used life cycle inventory parameter in this study is summarized in Table S4.

Table S5. Life cycle inventory parameters used in this study

Data set	Global warming impact (GWI)	Unit
Electricity		
Grid mix*	0.39[5]	ton CO_2-eq./MWh
LP steam	82.894[8]	kg CO_2-eq./GJ
Cooling water	Neglected	-
Hydrogen**	7.00[9]	ton CO_2-eq./ton
CO_2 (captured)	-0.71[5]	ton CO_2-eq./ton

*Electricity mix European Environment Agency (EEA).

**Considered compression process. 12.00 ton CO_2-eq. per ton H_2 via steam methane reforming.

7. Techno-economic analysis method

Techno-economic analysis (TEA) is a method to evaluate and analyze the techno-economic feasibility of a give process. Inside battery limits (ISBL) and outside battery limits (OSBL) method is used for the present analyses.[10] The annual operating cost is calculated as the sum of fixed and variable operating cost. The fixed capital investment (FCI) is estimated from the total equipment installation cost. All equipment installation costs are converted to 2019 prices in USD by considering the chemical engineering plant cost indexes (CEPCI). Capital expenditure (CAPEX) is described as following equations.

$$IEC = F_I \times FOB \qquad \text{* MERGEFORMAT (14)}$$

$$ISBL = IEC \times F_{ISBL} \qquad \text{* MERGEFORMAT (15)}$$

$$FCI = ISBL \times (1 + D\,\&\,E + X) \qquad \text{* MERGEFORMAT (16)}$$

$$OSBL = ISBL \times OS \qquad \text{* MERGEFORMAT (17)}$$

$$TPC = FCI + OSBL + WC \qquad \text{* MERGEFORMAT (18)}$$

where IEC is the installation cost; F_I is the installation factor; FOB is the equipment purchase cost; F_{ISBL} is the ISBL factor, which is calculated as the sum of piping, instrumentation and control, electrical system, civil, structure and building, and lagging and paint; $D\,\&\,E$ is the design and engineering factor; X is the contingency factor; OS is the offsite factor; WC is the working capital; TPC is the total plant cost (CAPEX).

The estimated CAPEX is converted to annualized investment cost using following equations.

$$AIC = TPC \times CRF \quad \text{* MERGEFORMAT (19)}$$

$$CRF = \frac{i(i+1)^n}{\left((i+1)^n - 1\right)} \quad \text{* MERGEFORMAT (20)}$$

where AIC is the annualized investment cost; CRF is the capital recovery factor; i is the annual discount rate; n is operation time of the system.

FOB for all equipment except for electrolyzer and PSA is estimated using literature.[10] The used purchased prices for electrolyzer, utility and raw material in this study is summarized in Table S5.

Table S6. Purchase prices used in this study

Data set		Value	Unit
Electrolyzer stack cost		112[11]	USD/kW
Electrolyzer BoP cost		303[11]	USD/kW
PSA unit[12]	Reference cost	1,989,043	USD
	Reference capacity	1,000	m^3/hr (flowrate)
	Scaling factor	0.7	-
CO_2 capturing cost		40[12]	USD/ton CO_2
Electricity		0.066[13]	USD/kWh
LP steam		6.08[7]	USD/GJ
Process water		0.15[6]	USD/m^3
O_2		95[13]	USD/ton
H_2		8,000[14]	USD/ton

8. Simulation results

Table S7. Simulation results for the CF-ECO_2R process. The simulation is conducted to predict the performance of the CF-ECO_2R process at operating voltages from 1.8 V to 2.3 V.

Operating voltage (V)	j_{CO} ($mAcm^{-2}$)	j_{H_2} ($mAcm^{-2}$)	FE_{co} (%)	CO_2 conversion (%)
1.8	14.3	0.5	92.6	4.7
1.9	30.0	1.0	93.6	9.5
2.0	62.7	2.0	97.1	18.9
2.1	131.1	4.1	95.5	35.5
2.2	223.7	8.2	92.9	55.6
2.3	249.5	16.4	88.6	62.9

9. References

1. X. Lu, D. Y. C. Leung, H. Z. Wang and J. Xuan, *Appl Energ*, 2018, **227**, 525-532.
2. H. Z. Wang, D. Y. C. Leung and J. Xuan, *Appl Energ*, 2013, **102**, 1057-1062.
3. Y. Kotb, S. E. K. Fateen, J. Albo and I. Ismail, *J Electrochem Soc*, 2017, **164**, E391-E400.
4. C. Georgopoulou, S. Jain, A. Agarwal, E. Rode, G. Dimopoulos, N. Sridhar and N. Kakalis, *Comput Chem Eng*, 2016, **93**, 160-170.
5. A. Sternberg, C. M. Jens and A. Bardow, *Green Chem*, 2017, **19**, 2244-2259.
6. R. Meys, A. Katelhon and A. Bardow, *Green Chem*, 2019, **21**, 3334-3342.
7. J. Lee, K. H. Ryu, H. Y. Ha, K. D. Jung and J. H. Lee, *J Co2 Util*, 2020, **37**, 113-121.
8. W. Chung, K. Roh and J. H. Lee, *Int J Greenh Gas Con*, 2018, **74**, 259-270.
9. E. Cetinkaya, I. Dincer and G. F. Naterer, *Int J Hydrogen Energ*, 2012, **37**, 2071-2080.
10. G. Towler and R. Sinnott, *Chemical engineering design: principles, practice and economics of plant and process design*, Elsevier, 2012.
11. A. T. Mayyas, M. F. Ruth, B. S. Pivovar, G. Bender and K. B. Wipke, *Manufacturing Cost Analysis for Proton Exchange Membrane Water Electrolyzers*, National Renewable Energy Lab.(NREL), Golden, CO (United States), 2019.
12. M. Jouny, W. Luc and F. Jiao, *Ind Eng Chem Res*, 2018, **57**, 2165-2177.
13. C. Hank, S. Gelpke, A. Schnabl, R. J. White, J. Full, N. Wiebe, T. Smolinka, A. Schaadt, H.-M. Henning and C. Hebling, *Sustain Energ Fuels*, 2018, **2**, 1244-1261.
14. S. Kimura and Y.Li, *ERIA Research Project Report FY2018 no.01*, ERIA, 2019, 140-183.