The design and operational space of syngas production via integrated direct air capture with gaseous CO2 electrolysis

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Abstract:

The overarching goal of limiting the increase in global temperature to ? 2.0? C likely requires both decarbonization and defossilization efforts. Direct air capture (DAC) and CO2 electrolysis stand out as promising technologies for capturing and utilizing atmospheric CO2. In this effort, we explore the details of designing and operating an integrated DAC-electrolysis process by examining some key parameters for economic feasibility. We evaluate the gross profit and net income to find the most appropriate capacity factor, average electricity price, syngas sale price, and CO2 taxes. Additionally, we study an optimistic scenario of CO2 electrolysis and perform a sensitivity analysis of the CO2 capture price to elucidate the impact of design decisions on the economic feasibility. Our findings underscore the necessity of design improvements of the CO2 electrolysis and DAC processes to achieve reasonable capacity factor and average electricity price limits. Notably, CO2 taxes and tax credits in the order of $400 per t-CO2 or greater are essential for the economic viability of the optimistic DAC-electrolysis route, especially at competitive syngas sale prices. This study serves as a foundation for further work on designing appropriate power system models that integrate well with the presented air-to-syngas route.

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Supplementary information: The design and operational space of syngas production via integrated direct air capture with gaseous CO_2 electrolysis

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S.1. Techno-economic assessment (TEA) calculations

S.2.1. Capital costs

To estimate the capital costs of direct air capture (DAC) equipment, we use two methods: the bare-module, Eq. S.1, and the Lang-factor, Eq. S.2, methods. The method of choice will depend on the cost information availability and source. On the other hand, we use \$233 per kWh in estimating the capital cost of electrolyzers, which was predicted by the H_2A production cost model [1] and is considered the state-of-the-art estimate today [2,3]. It is worth noting that previous estimates of CO_2 electrolyzers per m^2 vary significantly with a range of \$960-12,000 per m^2 [4–6]. Thus, we stick with the future estimate of the state-of-the-art H_2O electrolyzer CAPEX for both H_2O and CO_2 electrolyzers here. However, note that the capital costs of H_2O electrolyzers and CO_2 electrolyzers are equivalent to \$8,877 and \$4,713 per m^2, respectively, which fall within the wide range mentioned above.

(S.1) $$PEC = PEC_{old}\left(\frac{S_{new}}{S_{old}}\right)^n$$

(S.2) $$PEC = a + bS_{new}^n$$

In addition to estimating the equipment cost, the installation costs must be included in the total capital cost. We use the installation factors presented in Table S.1. to estimate these costs (Eq. S.3). Further, extrapolation to June 2023 costs was performed using the chemical engineering plant cost index (CEPCI), as shown by Eq. S.4, in which IEC_{old}, IEC_{2023}, $CEPCI_{old}$, and $CEPCI_{2023}$ are the IEC in the older year, IEC in June of 2023, CEPCI of the older year, and CEPCI of June 2023, respectively. We use a value of 803.3 for $CEPCI_{2023}$.

(S.3) $$IEC_{old} = f_{installation} \bullet PEC$$

(S.4) $$IEC_{2021} = IEC_{old} \bullet \left(\frac{CEPCI_{2023}}{CEPCI_{old}}\right)$$

Table S.1. Installation factors used in the present study.

Equipment	Installation Factor
Centrifugal fans	1.4

PVC packing	3.2
Pump	4
Crystallizer (pellet reactor)	2.2
Furnace (calciner)	2.5
Fluidized-bed dryer (slaker)	2.2
H_2O/CO_2 electrolyzer	1.2
Catalyst/membrane	1.2
Pressure swing adsorber	2.5

Moreover, we estimate the outside battery limit (OSBL), engineering, and contingency costs from the inside battery limit (ISBL) cost, Eq. S.5. We assume the OSBL is 40% of the ISBL, consistent with typical initial estimates of new petrochemical plants [7], and assume the engineering and contingency costs to be 10% and 30% of the combines ISBL and OSBL costs, respectively [7]. Finally, the fixed capital investment (FCI) or the capital expenditures (CAPEX) is the summation of ISBL, OSBL, engineering, and contingency costs, as shown by Eq. S.6. We use the capital recovery factor (CRF), Eq. S.7, to annualize the CAPEX, Eq. S.8, where i is the interest rate and t is the plant lifetime.

(S.5) $ISBL = \sum IEC_i$

(S.6) $FCI = CAPEX = ISBL + OSBL + Engineering + Contingency$

(S.7) $CRF = \frac{i(1+i)^t}{[(1+i)^t - 1]}$

(S.8) $Annual\ CAPEX = CAPEX \bullet CRF$

In the present work, the interest rate is assumed to be 7% for DACC and RWGS, and 10.1% for PEMWE and CO_2ER. The lifetime is assumed to be 25 years for DACC and RWGS, and 11 years for PEMWE and CO_2ER. Note that the electrolysis interest rate and lifetime is consistent with the 2020 H_2A production model for a future central PEM electrolysis system [1]. Similarly, the interest rates and lifetimes of DACC and RWGS are consistent with literature assumptions [8,9].

S.2.2. Operational costs

The operational costs are divided into fixed and variable operational costs ($OPEX_{fixed}$ and $OPEX_{var}$). $OPEX_{fixed}$ include the operating labor, supervision, direct salary overhead, maintenance, property taxes and insurance, rent of land, general plant overhead, and environmental charges [7]. Table S.2 summarizes how to calculate each of these factors. On the other hand, $OPEX_{var}$ include raw materials, utilities, and any consumable (e.g., catalysts), and Table S.3 summarizes the assumed prices of these elements. Finally, the total $OPEX_{annual}$ is the sum of $OPEX_{fixed}$ and $OPEX_{var}$, Eq. S.9.

(S.9) $$OPEX_{annual} = OPEX_{fixed} + OPEX_{var}$$

Table S.2. Assumptions of each operational cost component.

Component	Percentage	of
Supervision	25%	Operating labor
Direct salary overhead	50%	(Operating labor + Supervision)
Maintenance	3%	ISBL
Property taxes & insurance	1%	ISBL
Rent of land	1%	(ISBL + OSBL)
General plant overhead	50%	(labor + maintenance)
Allocated environmental charges	1%	(ISBL + OSBL)

Table S.3. Prices of components used in the techno-economic calculations.

Component	Price	Source/*Notes*
KOH ($/t)	450	Price of caustic potash in the U.S. in December of

		2020 based on data from ChemAnalyst [10]
$CaCO_3$ ($/t)	7	*Back calculated from discussion in* Keith et al. [8]
H_2O ($/t)	0.1	Keith et al. [8]
HCl ($/t)	84.77	Average 1-yr price in 2017-2018 based on data from Intratec [11]
Electricity ($/MWh)	45	*Rough average considering $30/MWh and $60/MWh are the minimum and maximum possible prices*
Natural gas ($/GJ)	5.03	Industrial natural gas price in the U.S. in 2021 [12]

S.2.3. Revenue

We assume the selling of syngas from the cathode and of O_2 from the anode of CO_2 electrolyzers. The price of syngas is a variable in our analysis, ranging from $0.3 to $1.0 per kg-syngas. However, we fixed the O_2 price to be $0.1 per kg-$O_2$ [13]. To estimate the revenue, we simply use Eq. S.10, where P_{O_2} and P_{syngas} are the prices of oxygen and syngas, $\dot{m}_{O_2}$ and $\dot{m}_{syngas}$ are the mass flow rates of oxygen and syngas, and CF is the capacity factor of the plant. Note that the final unit of the revenue must be $ per year, meaning that the mass flow rate should be in kg per year.

$$Revenue = \left(P_{O_2} \bullet \dot{m}_{O_2} + P_{syngas} \bullet \dot{m}_{syngas}\right) \bullet CF$$

S.2. Syngas market price

Table S.4. Literature-reported syngas prices.

Source	Price ($ per kg-syngas)
Pei et al.	0.01-0.04
Moreno-Gonzalez et al.	0.20
Daniel et al.	0.74
Almajed et al.	0.65

Using the average from several literature-reported values (Table S.4), we estimate the syngas market price to be:

$$P_{syngas,market} = \frac{\frac{0.01 + 0.04}{2} + 0.20 + 0.74 + 0.65}{4} = \$0.40\ per\ kg - syngas$$

S.3. Supplementary figures

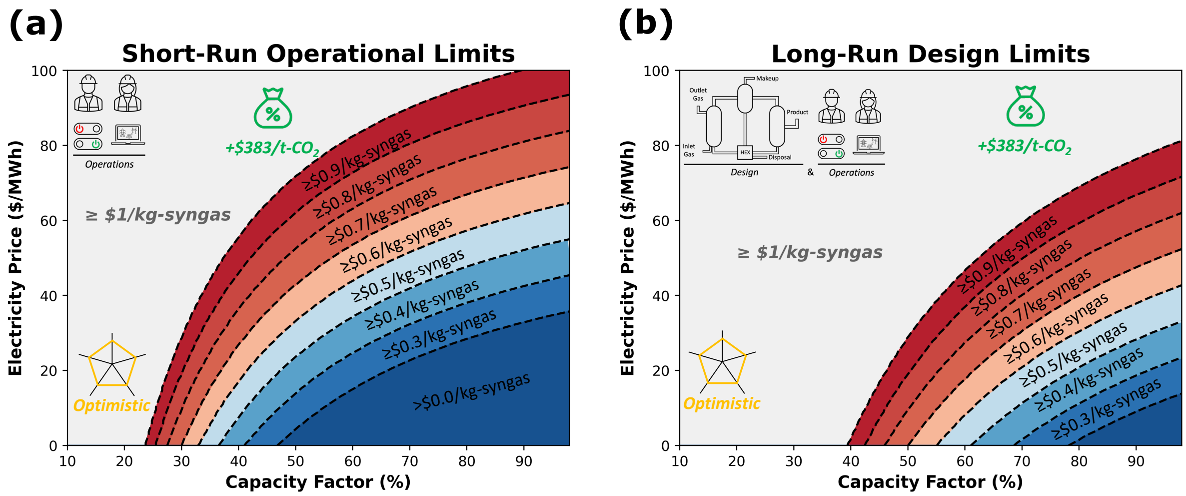

Figure S.1. Capacity factor and average electricity price limits for **(a)** positive gross profit and **(b)** positive net income at different syngas prices of the optimistic case (cell voltage = 2.0 V, current density = 1,500 mA per cm^2, FE_{CO} = 90%, CO_2 single-pass conversion = 27%) and with a $383 per t-$CO_2$ tax credit.

S.4. References

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