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The design and operational space of syngas production via integrated direct air capture with gaseous CO_2 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 CO_2 electrolysis stand out as promising technologies for capturing and utilizing atmospheric CO_2. 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 CO_2 taxes. Additionally, we study an optimistic scenario of CO_2 electrolysis and perform a sensitivity analysis of the CO_2 capture price to elucidate the impact of design decisions on the economic feasibility. Our findings underscore the necessity of design improvements of the CO_2 electrolysis and DAC processes to achieve reasonable capacity factor and average electricity price limits. Notably, CO_2 taxes and tax credits in the order of $400 per t-$CO_2$ 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.

Keywords: Carbon Dioxide Capture, Technoeconomic Analysis, Syngas, Aspen Plus, Modelling and Simulations.

1. INTRODUCTION

Suppressing the increase in global temperature to ≤ 2.0˚ C likely necessitates the combination of decarbonization and defossilization technologies, including point-source CO_2 capture (PSCC), carbon dioxide removal (CDR), CO_2 storage, and CO_2 utilization [1–7]. The path to carbon neutrality implies using defossilized carbon sources, such as biomass, sea/oceanwater, and air. There has been a significant effort on using biomass as a nature-based carbon source [8–10]. However, concerns have been raised about the effects of biomass-based technologies on crop prices, human rights, and their competition with food lands [3,11–15].

Alternatively, one could leverage sea/oceanwater and air as defossilized carbon sources. Indeed, a key CDR method that has been gaining significant attention in the recent years is direct ocean capture (DOC) [16–20], which benefits from the CO_2 equilibrium between the atmosphere and the ocean as a capture step and focuses on the extraction of CO_2 from carbonized oceanwater. Although this technology can be promising, it is still nascent and further research is underway to understand its potential in the broader scope of defossilization efforts.

Another key CDR technology is direct air capture (DAC), which captures CO_2 from the atmosphere using a chemical or a physical sorbent/solvent. DAC offers several advantages including smaller land requirements compared to nature-based CDR technologies, modular contactors, and almost no competition with food crop lands [7,21–23]. One of the advanced DAC designs utilizes a two-cycle process to capture CO_2 using a hydroxide-based solvent (generally, KOH) in the form of (bi)carbonates [24–27]. This technology is currently being developed and commercialized by a collaboration between Carbon Engineering and Oxy companies. However, one of the major challenges of hydroxide-based DAC is its high cost, with estimates ranging from $94 to $1,000 per t-$CO_2$, and high energy consumption, which ranges from 5.50 to 8.81 GJ per t-CO_2 [21,24,28–30]. Most of this high energy cost originates from the elevated temperature needed (900° C) to regenerate the captured CO_2 via calcination [30]. Nevertheless, hydroxide-based DAC is thought to be the most scalable and cost-effective DAC technology today [21,22], making it an attractive option for obtaining defossilized carbon from air.

To utilize this captured CO_2 in a way that achieves circularity, both thermochemical and electrochemical methods can be used to convert it to more valuable products such as syngas (i.e., a mixture of H_2 and CO), which is a key intermediate product that can be used in the production of methanol, ethylene, jet fuel, and other high-value products [31,32]. One of the most technologically mature methods for producing syngas from a feed of CO_2 is reverse water gas shift (RWGS), which takes in H_2 as a second reactant and produces syngas at a H_2:CO molar ratio of 1-2 [33,34]. The main downside of this technology is the high temperature (1,000° C) requirement that likely necessitates the use of traditional heat sources (e.g., natural gas).

An alternative technology is low-temperature CO_2 electrolysis, which directly utilizes electricity to reduce CO_2 to CO at ambient conditions over a silver electrocatalyst in the cathode of an electrochemical cell. Although still a nascent technology, low-temperature CO_2 electrolysis allows the direct utilization of renewable electrons, enabling the design of a fully renewable CO_2 utilization method. It is worth noting that several start-up and established companies are trying to develop and upscale this technology, including Twelve [35], GIGKarasek [36], Siemens [37], Evonik [37], and Dioxide Materials [38].

The integration of DAC with low-temperature CO_2 electrolysis (DAC-CO_2ER) can provide a promising defossilized air-to-syngas production pathway. We evaluated the techno-economics of this pathway against that of an integrated DAC-RWGS route in a previous effort [21], in which we found a potential route for DAC-CO_2ER to be economically competent with more conventional routes in a future scenario. One of the main takeaways was to operate CO_2 electrolysis at a current density of 1,500 mA per cm^2 and a cell voltage of ≤ 2.00 V to enable the competition between DAC-CO_2ER with DAC-RWGS and conventional methods for 2:1 syngas production.

In this work, we especially focus on the economic feasibility of the DAC-CO_2ER route that will allow it to be continuously operated at a large scale. We study the influence of capacity factor, average electricity price, syngas sale price, CO_2 taxes, and CO_2 tax credits on the process economics. We first estimate the design and operational limits of a baseline CO_2 electrolysis system by

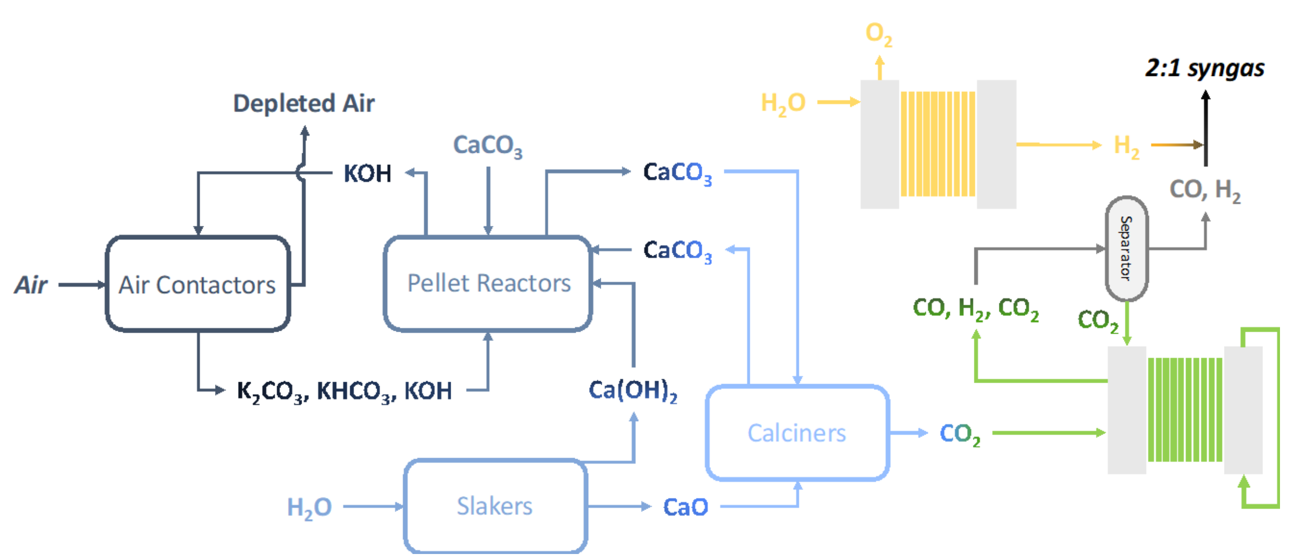

Figure 1. A block flow diagram of the process integration of DACC and CO_2 electrolysis. The blue blocks represent the units of the DACC plant, the green-colored electrolyzer is the CO_2 electrolyzer, and the yellow-colored electrolyzer is the proton exchange membrane water electrolyzer (PEMWE). We denote the pressure swing adsorption (PSA) unit as a separator in this figure.

varying the capacity factor, average electricity price, and syngas sale price. We then look at an optimistic case of CO_2 electrolysis to understand the effect of cell voltage and current density optimization on the design and operational limits. To expand on this, we perform a sensitivity analysis of the CO_2 capture cost on the optimistic-scenario limits to also consider further improvements of the DAC design. We then estimate the natural gas (NG) based market syngas sale price with CO_2 taxes, enabling a comparison with potential future conventional syngas prices. Finally, we add CO_2 tax credits to the DAC-electrolysis system to search for economically feasible regions of this defossilized syngas production pathway for design and operating conditions.

2. METHODOLOGY

2.1. Process description

Figure 1 envisions a block flow diagram of the presented defossilized syngas production pathway. The DAC technology considered here uses KOH to capture CO_2 from the atmosphere in the form of K_2CO_3 and $KHCO_3$ in an air contactor. The captured liquid solution is then sent to a set of pellet reactors along with a $Ca(OH)_2$ slurry to regenerate the liquid KOH solvent and produce $CaCO_3$ pellets. The pellets are then sent to calciners where they are dissociated into CaO and CO_2 at a temperature of 900° C. The CaO is then mixed with H_2O in a set of slakers to re-produce a $Ca(OH)_2$ slurry, whereas the gaseous product is dehydrated to produce a purified CO_2 stream. This whole process is continuous, allowing for the capture of CO_2 in the form of potassium (bi)carbonates as well as the regeneration of liquid KOH and gaseous CO_2.

The concentrated gaseous CO_2 can then be sent to a CO_2 electrolyzer where it is electrochemically reduced to CO using two electrons and two protons, Eq. (1). It is worth noting that the local pH near the catalyst surface determines the proton source, which also determines the reaction by-product (i.e., OH^- for neutral-to-alkaline local pH or H_2O for acidic local pH) [39]. In this work, we assume a high local pH, which corresponds to H_2O being used as the proton source. On the other side, the anode electrochemical reaction is assumed to be the oxygen evolution reaction (OER), Eq. (2), which commonly occurs on a Nickel-based or an Iridium-based electrocatalyst.

$$CO_2 + 2e^- + H_2O \rightarrow CO + 2OH^- \quad (1)$$

$$2OH^- \rightarrow \frac{1}{2}O_2 + H_2O + 2e^- \quad (2)$$

The CO_2 electrolyzer is not only producing CO, but also H_2 via the competing hydrogen evolution reaction (HER), Eq. (3). However, the CO_2 electrolyzer is generally optimized to increase the CO selectivity and decrease the H_2 selectivity in the product stream. Thus, we supply additional H_2 from a proton exchange membrane water electrolyzer (PEMWE) that oxidizes H_2O to produce O_2 and protons (H^+), Eq. (4). The protons then pass a cation exchange membrane (CEM) as they travel to the cathode side to be electrochemically reduced to H_2 via HER, Eq. (3).

$$2H^+ + 2e^- \rightarrow H_2 \quad (3)$$

$$H_2O \rightarrow 2e^- + \frac{1}{2}O_2 + 2H^+ \quad (4)$$

2.2. Process models

A hydroxide-based DAC plant was modeled in Aspen Plus based off of Keith et al.'s design [24]. This model provides the mass and energy balances required to estimate the equipment and operational costs of the plant. In addition, we use our own CO_2 electrolysis model that calculates the mass and energy balances of a specified electrolysis system. For further details about the process models, we refer the reader to our previous publication [21].

We design the CO_2 electrolysis system based off of Wen and Ren et al.'s experimental results that achieved 90% Faradaic efficiency of CO (FE_{CO}) at 612 mA per cm^2 and 3.3 V (energy efficiency (EE) ≈ 40%) in a 400-cm^2, 4-cell electrolyzer stack [40]. These performance values are used in our baseline scenario (Table 1). We additionally consider an optimistic scenario in which we assume achievement of a current density and a cell voltage of 1,500 mA per cm^2 and 2.0 V (EE ≈ 67%), respectively. Table 1 summarizes these assumptions.

Table 1. Key baseline and optimistic assumptions of CO_2 electrolysis.

Metric	Baseline	Optimistic
Symbol		
Total Current Density (mA per cm^2)	612	1,500
Cell Voltage (V)	3.3	2.0
FE_{CO}	90%	90%
Single-Pass Conversion	27%	27%

2.3. Techno-economic model

Our techno-economic model was developed to take the results of our process models as inputs and estimate the equipment and operational costs according to Towler and Sinnot's methodology [41]. In addition, we estimate the gross profit, Eq. (5), and the net income, Eq. (6), while varying the capacity factor and average electricity price at a constant syngas price. The gross profit is used as an indicator of the system operations whereas the net income is used as an indicator of both the design and operation of the system. In Eq. (5) and (6), OPEX, CAPEX, and CRF refer to operational cost, capital cost, and capital recovery factor, respectively. The CRF, Eq. (7), is used

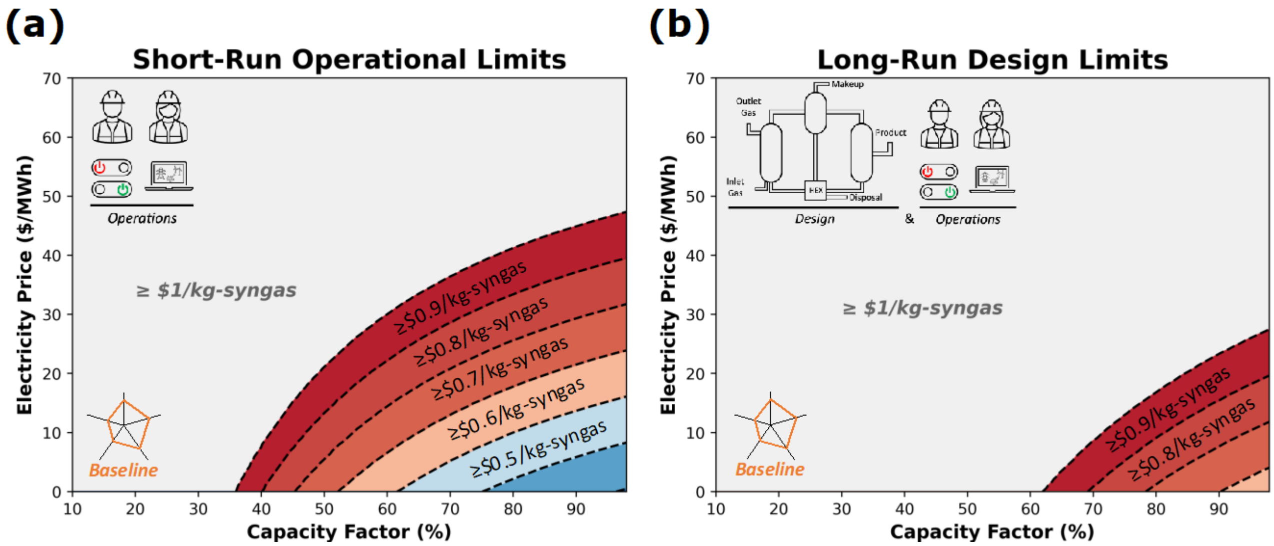

Figure 2. Capacity factor and average electricity price limits for **(a)** positive gross profit and **(b)** positive net income at different syngas prices of the baseline case (cell voltage = 3.3 V, current density = 612 mA per cm^2, FE_{CO} = 90%, CO_2 single-pass conversion = 27%).

to annualize the capital cost of the system, where i is the interest rate and N is the plant lifetime. For key assumptions and further details about our techno-economic model, we refer the reader to the SI.

$$Gross\ Profit = Revenue - OPEX \quad (5)$$

$$Annual\ Net\ Income = Gross\ Profit - CAPEX \bullet CRF \quad (6)$$

$$CRF = \frac{[i(1+i)^N]}{[(1+i)^N - 1]} \quad (7)$$

We use the techno-economic model outputs to define realistic targets for future renewably powered CO_2 electrolysis designs and techno-economic evaluations, especially in the context of renewably driven defossilized air-to-syngas pathways.

3. RESULTS & DISCUSSION

Two of the key assumed parameters in techno-economic assessment (TEA) calculations in electrolysis are the capacity factor and the average electricity price. In the past, a capacity factor of ≥ 90% and an average electricity price in the range of $20-60 per MWh have been used in the CO_2 electrolysis field [21,42–47]. Such values are highly optimistic for interactions with a highly renewable decarbonized power system and might unrealistically benefit the economics of CO_2 electrolysis. To provide more realistic assumptions, a more-detailed power system model is needed to fill this gap. However, before this is pursued, it is important to understand the combinations of the capacity factor, average electricity price, syngas sale price, and CO_2 taxes that would allow the whole route to generate positive gross profit and positive net income.

We consider two cases in this effort. In the first case, we focus on the operational limits of the presented DAC-electrolysis route (Fig. 1) by estimating the gross profit while varying the capacity factor and the average electricity price at syngas sale prices of $0.3-1.0 per kg-syngas. We then identify the minimum capacity factor and average electricity price at each syngas price that allow the gross profit to stay positive. In the second case, we take the plant's design into consideration as well, meaning that we not only focus on the short-term economic decisions but the long-term ones as well. To accomplish this, we estimate the same parameters that enable the net income to stay positive at the different syngas sale prices. We conduct the same analysis for four scenarios: 1) Baseline without CO_2 tax credits (Fig. 2a and 2b), 2) Optimistic without CO_2 tax credits (Fig. 3a and 3b), 3) Baseline with a CO_2 tax credit of $130 per t-$CO_2$ (Fig. 5a and 5b), and 4) Optimistic with a CO_2 tax credit of $130 per t-$CO_2$ (Fig. 5c and 5d).

3.1. Design and operational economic limits of the baseline DAC-CO_2ER route without CO_2 tax credits

Figures 2a and 2b show the relationship between the capacity factor and the average electricity price at different syngas prices that would allow the gross profit and net income to be positive, respectively. We observe that a positive gross profit (Fig. 2a) at lower syngas prices requires a high-capacity factor and a low average electricity price. As the assumed syngas sale price increases from $0.3 to $1.0 per kg-syngas, more flexibility in the capacity factor and the average electricity price can be obtained, while remaining economically viable. For instance, at an assumed syngas sale price of $0.7 per kg-

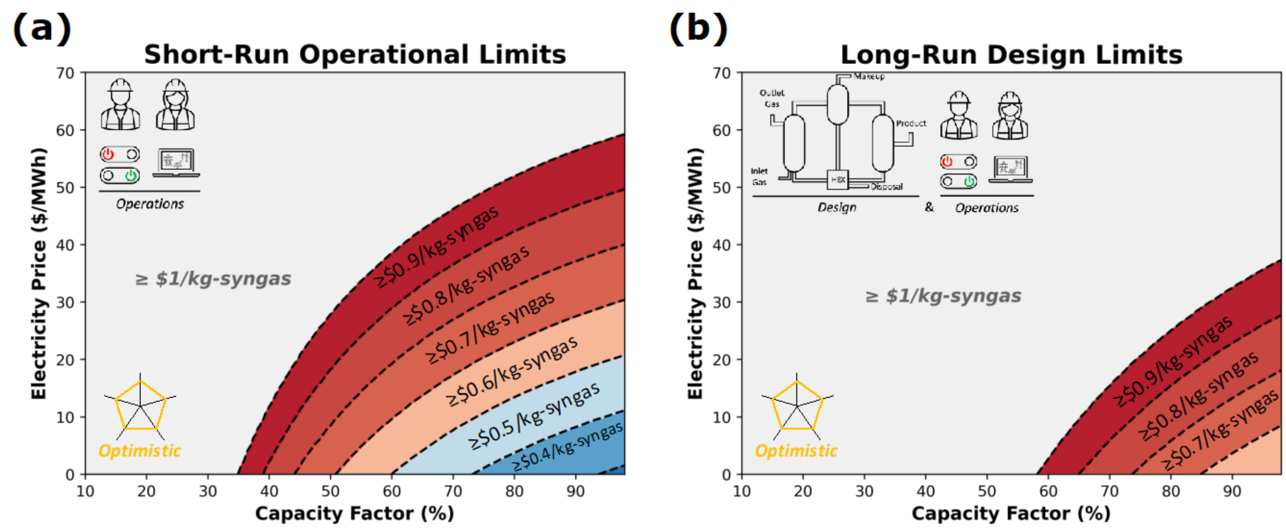

Figure 3. Capacity factor and average electricity price limits for **(a)** positive gross profit and **(b)** positive net income at different syngas prices of the optimistic case (cell voltage = 2.0 V, current density = 1,500 mA per cm^2, FE_{CO} = 90%, CO_2 single-pass conversion = 27%).

syngas, a capacity factor of ≥ 95% is required at an average electricity price of $23 per MWh to generate a positive gross profit. However, at a higher assumed syngas sale price of $1.0 per kg-syngas, more operational flexibility can be provided (e.g., capacity factor of 50%) at the same average electricity price ($23 per MWh), while still generating a positive gross profit. This finding demonstrates the importance of capacity factor and average electricity price assumptions in determining the short-term operational economic feasibility of the investigated DAC-electrolysis route.

At longer timescales, the cost associated with the design of the plant (e.g., equipment, instrumentations) must be considered. We observe a red shift of the colormap that requires higher syngas prices at higher capacity factors and lower average electricity prices (Fig. 2b). This is caused by the addition of the annualized capital costs, which adds an economic restriction on the design and operations of the plant that must be considered and minimized at an early stage. However, it is worth noting that, in practice, this restriction does not impact the operational decisions but rather the design decisions.

Indeed, reducing the capital cost could significantly help achieve more flexible operations of the electrolysis unit such that the DAC-electrolysis route stays economically feasible throughout the broad range of dynamic electricity prices anticipated in the future [48]. Additionally, benefitting from incentives [49] that partially or fully pay off the capital cost of the plant could significantly hasten the deployment of these defossilized pathways, especially when considering the current average syngas market price ($0.40 per kg-syngas, see the discussion in section 3.4 and calculation in the SI). However, it is worthwhile to re-iterate that this restriction does not influence the operational decisions of the plant.

3.2. Design and operational economic limits of the optimistic DAC-CO_2ER route without CO_2 tax credits

Improving the design of CO_2 electrolyzers such that they achieve high current densities (≥ 1,500 mA per cm^2) at low cell voltages (≤ 2.0 V; EE ≥ 67%) is still in progress [21,50]. Defining research targets that consider the economics of such pathways would be helpful to CO_2 electrolysis researchers at this developmental stage. Figure 3 shows the same relationships from Figure 2, however considering an optimistic CO_2 electrolysis performance that achieves 1,500 mA per cm^2 at 2.0 V (EE ≈ 67%).

We find the average electricity price to gain more flexibility when considering the optimistic CO_2 electrolysis performance in our gross profit calculations (Fig. 3a). For instance, at an assumed syngas sale price of $1.0 per kg-syngas, the maximum average electricity prices for the baseline and optimistic scenarios that enable positive gross profits at a capacity factor of 70% are approximately $37 and $46 per MWh, respectively. This finding is mainly due to the large influence of electricity costs on the economics of DAC-electrolysis routes, as driven by the cell voltage (or energy efficiency) [21,50].

In addition, we find the capacity factor limits of maintaining a positive gross profit to also change as the cell voltage and current density are optimized (Fig. 3a). At an average electricity price of $30 per MWh and an assumed syngas sale price of $1.0 per kg-syngas, the capacity factor limits of the baseline and optimistic scenarios that allow positive gross profits are estimated to be 60% and 52%, respectively. The higher flexibility with operating at lower capacity factors while still generating a positive gross profit in the optimistic scenario is also driven by the lower electricity costs, which originate from achieving a lower cell voltage of 2.0 V.

Similarly, Figure 3b shows the same general results–i.e., higher flexibility of the average electricity price and the capacity factor limits to generating a positive net income. However, we observe a slightly higher flexibility in the capacity factor, resulting from the reduction of the cell voltage that reduces the power of the electrolyzer; and thus, the electrolyzer's capital cost. Therefore, higher flexibility in the capacity factor can be obtained in the optimistic scenario for operating with a positive net income.

Although assuming an optimistic scenario provides more flexibility in the average electricity price and capacity factor, high syngas prices of ≥ \$0.6 per kg-syngas are still needed to generate positive gross profit and net income (Fig. 3). In the following sections, we will explore the effect of CO_2 capture costs, CO_2 taxation on emitting technologies, and CO_2 tax credits for capture technologies in order for the current projections of the integrated process to make economic sense.

3.3. Design limits at different CO_2 capture costs without CO_2 tax credits

Sourcing the CO_2 from flue gases or from other non-fossil sources could have a significant influence on the economic feasibility of the presented syngas production route. Thus, we estimated the long-run design limits at different capture costs ranging from \$0 to \$250 per t-CO_2, as shown in Figure 4.

In general, as the CO_2 capture cost increases, the plot shifts to the red region. At a CO_2 capture cost of \$100 per t-CO_2, consistent with the U.S. department of energy (DOE) carbon shot goals, we find the average electricity price to be \$19 per MWh at a capacity factor of 80% and a syngas sale price of \$0.7 per kg-syngas. Reducing the CO_2 capture cost to \$50 per t-CO_2, consistent with sourcing CO_2 from PSCC, allows more flexibility in the average electricity price (≤ \$25 per MWh) at the same capacity factor and syngas sale price. This result demonstrates the importance of reducing the CO_2 capture cost to less than \$100 per t-CO_2 or sourcing the CO_2 from an alternative source that would provide the carbon at a cheaper price. However, herein, we continue to focus on DAC to present an environmental process that allows the production of 2:1 syngas from air.

3.4. Conventional syngas market price with CO_2 taxation

The market syngas price is an important metric to compare against when evaluating emerging syngas production pathways. Previous literature have cited or estimated different syngas prices from natural gas (NG) feedstock processes, ranging from \$0.03 to \$0.74 per

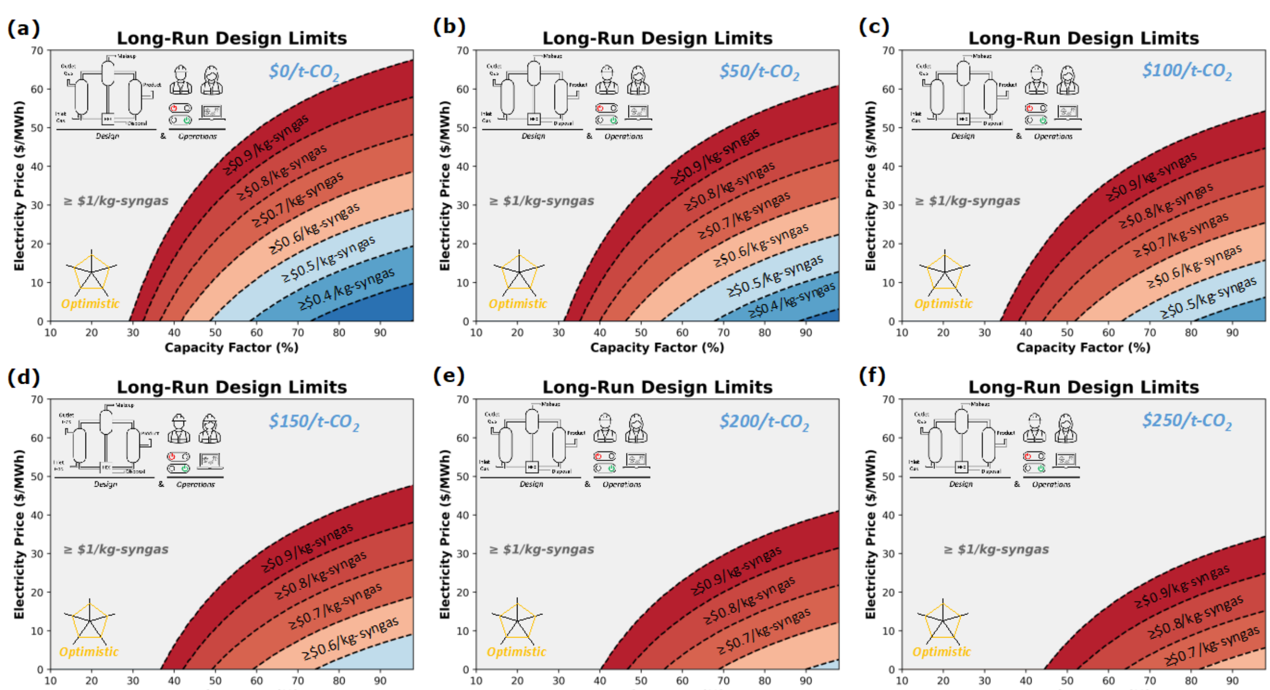

Figure 4. (a-f) Capacity factor and average electricity price limits for positive net income at different syngas prices of the optimistic case (cell voltage = 2.0 V, current density = 1,500 mA per cm^2, FE_{CO} = 90%, CO_2 single-pass conversion = 27%) and at various CO_2 capture prices ranging from \$0 to \$250 per t-CO_2.

kg-syngas [21,33,44,51,52]. We use the average NG-based syngas price of these estimates as the market price in our analysis. We assume a NG-based plant that is composed of dry methane reforming (DMR) for 1:1 syngas production and steam methane reforming (SMR) for additional H_2 supply to produce 2:1 H_2:CO syngas, according to the design of Rezaei and Dzuryk [33]. Figure 5 shows the re-calculated NG-based syngas price with CO_2 taxes of \$0-550 per t-CO_2. We assume a 90% capacity factor to estimate the process and energy-associated CO_2 emissions from the SMR-DMR pathway. Note that we are not accounting for any emissions outside the scope of the SMR-DMR process (e.g., natural gas processing).

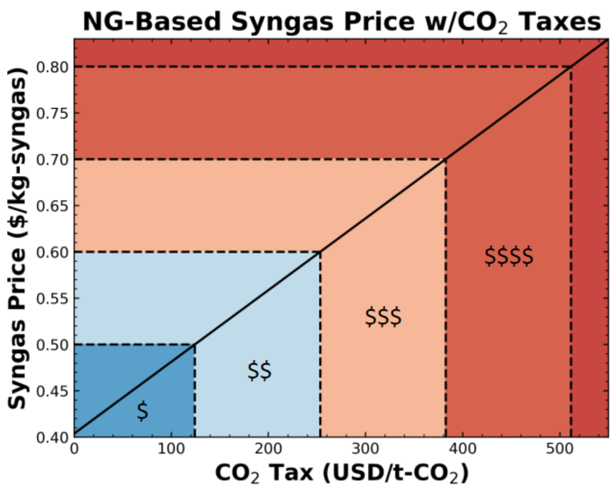

Figure 5. NG-based syngas price as a function of CO_2 taxes. The color codes from blue (\$) to orange (\$\$\$\$) correspond to the ranges ≤\$0.5, ≤\$0.6, ≤0.7, and ≤\$0.8 per kg-syngas cases, respectively. Note that we are not performing a full life-cycle assessment here; we are only accounting for the emissions from the DMR-SMR process, ignoring the emissions associated with raw materials' processing.

The linear relationship shows that the syngas price would increase to \$0.79 per kg-syngas with a CO_2 tax of \$500 per t-CO_2. Although this would give the DAC-electrolysis pathway more flexibility in the capacity factor and average electricity price choices, it suggests a CO_2 tax that is three times higher than the highest CO_2 tax implemented today (\$155 per t-CO_2 in Uruguay [53]). Thus, it is likely not realistic to consider reaching a CO_2 tax rate of \$500 per t-CO_2 by mid-century.

However, considering a CO_2 tax rate of \$155 per t-CO_2, the re-calculated NG-based syngas price increases from \$0.40 to approximately \$0.53 per kg-syngas (Fig. 5). At this price, the gross profit of the baseline and optimistic cases can be positive, although at restrictive capacity factor and average electricity price values, whereas the net income can only be negative. The only exception to this conclusion is if the CO_2 capture costs dropped to ≤ \$100 per t-CO_2, assuming no tax credits are provided to CO_2 capture (note that we will explore CO_2 tax credits in the next section). This finding, along with our previous results [21], suggest that a capital cost reduction of electrolyzers and air contactors would be necessary to make the economics of DAC-electrolysis viable. In addition, deployment incentives that partially or fully pay the capital expenses of building DAC-electrolysis plants could make a difference in deploying such emerging technologies and allowing them to compete with existing NG-based syngas production methods. In parallel, CO_2 tax credits could enormously help the net income to become positive by paying off some of the annual capital cost payments.

3.5. Design and operational economic limits of the baseline and optimistic DAC-CO_2ER route with a CO_2 tax credit of \$130 per t-CO_2

CO_2 tax credits can be paid to CO_2 capture plants whether they capture the gas from point sources or from air. In the U.S., the 45Q tax credit code [49] pays DAC plants a tax credit of \$180 per tonne of captured and geologically stored CO_2, and \$130 per tonne of captured and used CO_2. In our analysis, we therefore use a CO_2 tax credit of \$130 per t-CO_2 for the captured CO_2 by DAC to be used in the production of 2:1 syngas.

Figure 6 shows the capacity factor and average electricity price limits of the baseline (Fig. 6a and 6b) and optimistic (Fig. 6c and 6d) CO_2 electrolyzer cases with a CO_2 tax credit of \$130 per t-CO_2. The optimistic case enables more flexibility in the capacity factor and average electricity price at all syngas prices. For example, a price of \$0.70 per kg-syngas at a capacity factor of 80% can generate a positive gross profit at average electricity prices of ≤ \$32 and ≤ \$40 per MWh for the baseline and optimistic cases, respectively. For the same case and same conditions, the maximum average electricity price lowers to \$7 and \$13 per MWh for the two cases, respectively, to generate a positive net income. These results clarify that a CO_2 tax of \$155 per t-CO_2 and a CO_2 tax credit of \$130 per t-CO_2 are insufficient for the considered DAC-electrolysis route to be economically feasible, especially when considering annual capital cost payments.

For the optimistic case to generate positive gross profit and net income at a reasonable average electricity price and competitive syngas sale price, two conditions must be met. First, a higher tax rate implemented on NG-based syngas production is necessary. For instance, a CO_2 tax rate of \$383 per t-CO_2 would increase the syngas market sale price to \$0.70 per kg-syngas, as shown in Figure 5. This rate is more than double the highest CO_2 tax rate today–\$155 per t-CO_2–but is necessary from a business standpoint to strengthen the economic competition of the presented syngas production pathway.

Second, the CO_2 tax credits must be increased. Assuming an equal CO_2 tax credit of $383 per t-$CO_2$, the average electricity price limit of the optimistic scenario at a syngas price of $0.70 per kg can increase from $4 to $47 per MWh to generate a positive net income, while staying at a 90% capacity factor limit (Fig. S.1b). At this average electricity price and scenario, there will be more freedom in the operational decisions because the gross profit can stay positive even at a low-capacity factor of 60%, albeit at an average electricity price of $18 per MWh (Fig. S.1a). Although discouraged from a design perspective, this scenario would allow the continued and economic operation of the plant.

To put these results into context, NREL's annual technology baseline (ATB) analysis predicts a levelized cost of energy (LCOE) of utility-scale solar PV with battery storage in the range of $35-90 per MWh in 2050 [54]. The analysis presented in this section highlights the economic and policy challenges faced by the presented DAC-electrolysis pathway. In other words, it will be difficult for the DAC-electrolysis system to compete with conventional syngas production methods without a CO_2 emission tax rate and a CO_2 capture tax credit on the order of $400 per t-$CO_2$. Even in this scenario, the plant must operate most of the year at a capacity factor of ≥ 80% and the average electricity price must be in the lower range of the NREL ATB's LCOE predictions (i.e., ≤ $40 per MWh). Thus, further design and energy efficiency improvements as well as policy incentives are necessary before this pathway can be commercialized at scale.

4. SUMMARY AND FUTURE TARGETS

In this work, we focused on the capacity factor and average electricity price limits at several syngas prices that enable the gross profit and net income of a DAC-electrolysis route to be positive. We considered hydroxide-based DAC as well as gaseous CO_2 and liquid PEM H_2O electrolysis systems to produce 2:1 H_2:CO syngas. We additionally considered an SMR-DMR conventional route to re-calculate the syngas price after the addition of CO_2 taxes. We analyzed baseline and optimistic scenarios of CO_2 electrolysis and accounted for a tax credit payment of $130 per t-$CO_2$.

Our findings suggest that deploying the presented DAC-electrolysis route for syngas production will be economically challenging, even after considering current CO_2 taxes and tax credits. Indeed, our results show that the very best-case scenario–which considers improved CO_2 electrolysis performance, a CO_2 tax rate and tax credit of $383 per t-$CO_2$, and a capacity factor of ≥ 80%–still requires an average electricity price of $40 per MWh to generate both positive gross profit and net income. This price is in the lower range of the 2050 LCOE predicted average electricity prices by NREL's ATB analysis for a utility-scale solar PV with battery storage, and it is about 33% lower than the average 2023 wholesale electricity prices in U.S. markets [55]. Thus, several targets must be pursued before this pathway can be deployed as a defossilized syngas production route.

For CO_2 electrolysis, the main challenge is to achieve high current densities (≥ 1,500 mA per cm^2) at low cell voltages (≤ 2.00 V) to lower the capital cost while improving the energy efficiency of the process. However, special attention must be paid to the durability and stability of the electrolysis system as achieving the performance metric without stability would not allow industrial deployment at the high capacity factors required for profitability [56]. In addition, flexible operation is still an open problem in the low-temperature CO_2 electrolysis field, requiring experimental tests of interrupted electrolysis operations for long durations.

Hydroxide-based DAC plant designs must also be optimized to lower the energy consumption and capital costs. Specifically, the air contactor capital cost needs to be reduced to maximize the net income of the entire integrated route. Alternative low-temperature regeneration methods could help reduce the capital cost as there would not be any need to using heat exchanger networks, which accounts for approximately 21% of the total capital cost of the presented route [21].

Outside of technology development, high carbon taxes on CO_2-emitting technologies and high carbon tax credits for CO_2-capturing technologies would likely be necessary. Our results highlighted the importance of these policies in the shift from fossil-based to fossil-free production of syngas. For the defossilized air-to-syngas route presented here to be economically viable, CO_2 taxes and tax credit on the order of $400 per t-$CO_2$ are required. These numbers are unquestionably too high. However, early and fast deployment is necessary to enable learning-by-doing and economies-of-scale to help reduce the total cost of these emerging defossilized pathways; and thus, their required CO_2 taxes and tax credits.

Future work should explore several avenues, one of which is the integration of a detailed power system model that considers the dynamics of renewable electricity generation and prices as well as energy storage. In this avenue, a comparison with wholesale electricity supply should be considered to understand the best-case scenario for the DAC-electrolysis route to be economically feasible. In addition, alternative air-to-syngas routes should be explored with a similar methodology as presented here. Indeed, the most feasible integrated air-to-syngas design is still unknown, motivating future works to further explore this research path.

Finally, it is worthwhile to note that the present

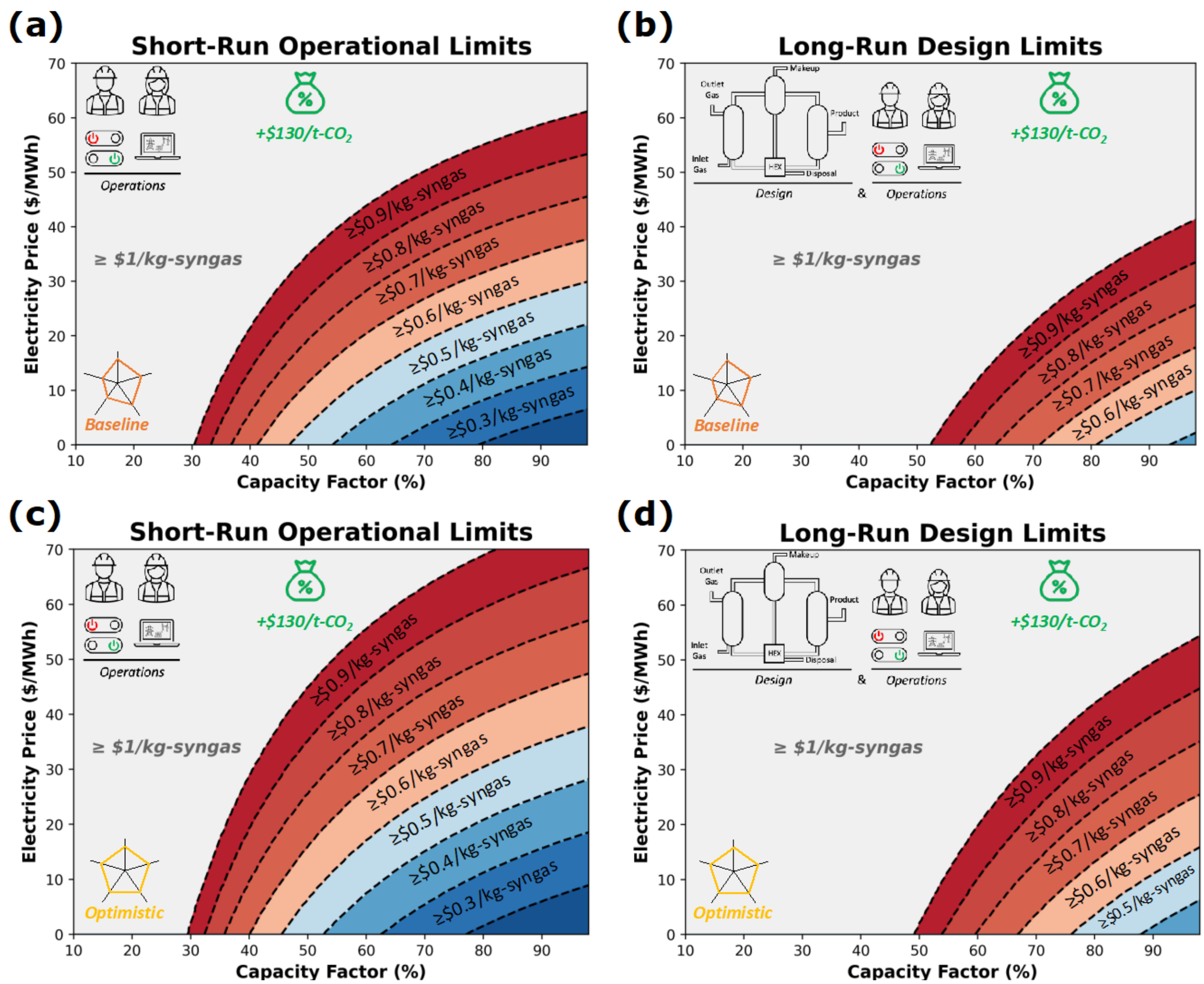

Figure 6. Capacity factor and average electricity price limits for **(a)** positive gross profit and **(b)** positive net income at different syngas prices with a CO_2 tax credit of \$130 per t-CO_2 of the baseline case. **(c)** and **(d)** are the same limits with the same CO_2 tax credit but for the optimistic case (cell voltage = 2.0 V, current density = 1,500 mA per cm^2, FE_{CO} = 90%, CO_2 single-pass conversion = 27%).

study particularly considered sourcing CO_2 from air. However, there are other sources of CO_2, such as the ocean, flue gases, and CO_2 process emissions, which were not explored here. Specifically, the latter two sources are likely to enhance the process economics of the whole integrated pathway, potentially allowing stronger competition with conventional NG-based syngas production methods. However, one should be careful with environmental concerns of upstream processes that generate these point-source gases to assure the design of a sustainable, circular, and environmental process for syngas production.

DIGITAL SUPPLEMENTARY MATERIAL

The supplementary information file includes details about the techno-economic assessment calculations and supplementary figures.

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