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Economic and Environmental Barriers of CO₂-Based Fischer–Tropsch Electro-Diesel

Juan D. Medrano-García, Margarita A. Charalambous, and Gonzalo Guillén-Gosálbez*

ABSTRACT: Electro-fuels are seen as a promising alternative to curb carbon emissions in the transport sector due to their appealing properties, similar to those of their fossil counterparts, allowing them to use current infrastructure and state-of-the-art automotive technologies. However, their broad implications beyond climate change remain unclear as previous studies mainly focused on analyzing their carbon footprint. To fill this gap, here, we evaluated the environmental and economic impact of Fischer–Tropsch electro-diesel (FT e-diesel) synthesized from electrolytic H₂ and captured CO₂. We consider various power (wind, solar, nuclear, or the current mix) and carbon sources (capture from the air (DAC) or a coal power plant) while covering a range of impacts on human health, ecosystems, and resources. Applying process simulation and life cycle assessment (LCA), we found that producing e-diesel from wind and nuclear H₂ combined with DAC CO₂ could reduce the carbon footprint relative to fossil diesel, leading to burden-shifting in human health and ecosystems. Also, it would incur prohibitive costs, even when considering externalities (i.e., indirect costs of environmental impacts). Overall, this work highlights the need to embrace environmental impacts beyond climate change in the analysis of alternative fuels and raises concerns about the environmental appeal of electro-fuels.

KEYWORDS: Fischer-Tropsch synthesis, electro-fuels, electro-diesel, direct air capture (DAC), life cycle assessment (LCA), global warming, externalities, burden-shifting

INTRODUCTION

Diesel is a refined product of crude oil used in compression-ignition internal combustion engines to provide power for the transportation and energy sectors. The total diesel demand amounted to 86 EJ/y in 2018,¹ most of which was used in trucks and ships to transport goods and the manufacturing sector. The transportation sector alone emitted 8.19 Gt of CO₂ in 2019 (24% of global GHG emissions), contributing to air pollution with substances like nitrogen oxides (NOₓ) and particulate matter (PM₂.₅) that are particularly detrimental to human health.²,³ Under current policies designed to reach carbon-neutrality by 2050,⁴ there is a strong motivation to replace diesel with more sustainable alternatives. Nevertheless, the good properties of diesel and the current optimized vehicle fleet for this fuel will make the transition particularly challenging.

As a substitute for fossil diesel, electro-diesel (e-diesel) is particularly appealing due to its high “drop-in” quality. It has the highest energy density per kilometer among all alternative fuels and similar characteristics to those displayed by fossil diesel. Notably, Fischer-Tropsch (FT) diesel could be integrated into existing infrastructure with minor changes while reducing pollutant emissions.⁵ Moreover, the high cetane number improves engine efficiency, enabling a fast market penetration.⁶

The FT process relies on a heterogeneously catalyzed pathway to convert syngas to liquid hydrocarbons. The products encompass a variety of simple hydrocarbon chains of different lengths, depending on the process conditions.⁶,⁷ The synthesis and implications of FT fuels have been extensively studied. However, substantial literature is based on biomass, with only a few works considering using captured CO₂ and electrolytic H₂ as feedstock. Furthermore, many of these studies focus on economic performance, disregarding environmental impacts⁸ or at most quantifying only the global warming potential while omitting other metrics.¹⁴–¹⁷

Focusing on biomass-based FT fuels, Swanson et al. studied the gasification of corn stover to produce FT-gasoline, achieving production costs of 1.06–1.32 $/L.¹⁸ Martin and...
Grossmann optimized a process superstructure for the synthesis of FT-diesel from lignocellulosic switchgrass, yielding a potential production cost of 0.75 $/gal. Cuéllar-Franca et al. performed an economic and environmental analysis of four FT configurations based on sewage sludge diesel covering 11 LCA metrics. They concluded that, even in the best economic scenarios, costs were 4 times higher than in fossil diesel (1.85−3.00 £/L vs 0.44 £/L), while the FT fuel outperformed fossil diesel in all the LCA metrics except for global warming and ozone depletion, being the former in the range of 3.2−17.2 kg CO$_2$-eq/L fuel. Ben Hnich et al. found that FT palm oil diesel and gasoline could outperform their fossil counterparts in both global warming (7.65 kg CO$_2$-eq/GJ) and resource scarcity (28.58 kg oil-eq) while worsening other environmental categories such as fine particulate matter formation, freshwater eutrophication, and terrestrial acidification. Similarly, Okeke et al. studied FT miscanthus diesel finding that it could decrease slightly carcinogenic, noncarcinogenic, and ecotoxicity, relative to the fossil analog, while massively increasing ozone depletion, smog, acidification, eutrophication, and respiratory effects.

Concerning electro-fuels, Isaacs et al. recently studied their production from CO$_2$ captured from air coupled with H$_2$ either from proton exchange membrane (PEM) electrolysis, or in tandem with biomass gasification in the United States. Analyzing two electricity and three biogenic H$_2$ sources, they found that wind energy outperforms solar in carbon dioxide equivalent (CO$_2$-eq) emissions, while a synergistic combination of both provides the best economic result. Samavati et al. studied a solid oxide electrolyzer cell (SOEC) implementing co-electrolysis coupled with biomass gasification. They concluded that this e-fuel is economically uncompetitive but can curb carbon emissions by 98−102%. The same authors also reported that increasing the share of electrolytic H$_2$ results in higher fuel costs and greenhouse gas emission savings. Liu et al. studied the environmental implications of using direct air capture CO$_2$ in FT e-fuel, finding that its climate change impact was way below that of fossil diesel considering its final combustion (28−12 g CO$_2$-eq/MJ e-fuel vs 104 g CO$_2$-eq/MJ diesel). Finally, the synthesis of FT e-diesel from direct air-captured CO$_2$ and a hybrid wind/solar electricity fueled alkaline electrolyzer (AEC) for H$_2$ production was studied by Fasihi et al., who by considering O$_2$ valorization, managed to reach production costs as low as 0.69 €/L of e-diesel.

In general, all of these studies concluded that FT e-diesel is economically unappealing, although it can reduce the climate change impact of fossil diesel substantially. However, its performance on impacts beyond global warming remains unclear because they are often omitted. This simplification is critical because electro-fuels may shift environmental burdens to other categories. Notably, this collateral damage has been observed in biomass-based synthetic fuels.
carbon power mixes,\textsuperscript{22,23} carbon capture and utilization,\textsuperscript{24,25} and FT electro-gasoline,\textsuperscript{26} to mention a few. Quantifying these potential adverse effects of electro-fuels is considered critical for designing optimal technological roadmaps for the transport sector. Given the lack of environmental information beyond global warming reported on FT e-diesel, we analyzed the full implications of its production under different electricity and CO\textsubscript{2} source scenarios.

Here, we carried out a complete environmental and economic assessment of FT e-diesel from renewable H\textsubscript{2} and captured CO\textsubscript{2} to shed light on the potential occurrence of burden-shifting. We found that using CO\textsubscript{2} from direct air capture provides the largest carbon emissions savings, while CO\textsubscript{2} from coal power plants leads to the lowest costs. Furthermore, nuclear and wind electricity lead to the lowest carbon footprint and cost, respectively. However, e-diesel is also found to shift environmental burdens to human health and ecosystems, which raises concerns about its large-scale deployment.

\section*{METHODS}

To carry out our assessment, we developed a process simulation of the FT plant based on a PEM electrolyzer in Aspen HYSYS v11. We considered four different electricity sources and two types of CO\textsubscript{2} from direct air capture (DAC) and coal power plant capture (COAL), leading to eight scenarios, as shown in Figure 1. Based on the simulation results (inputs and outputs), we carried out a life cycle assessment (LCA) in SimaPro v9.2\textsuperscript{27} using Ecoinvent v3.5.\textsuperscript{28} Finally, we performed a standard economic assessment considering CAPEX and OPEX expenditures.\textsuperscript{29} We present first the alternative scenarios, followed by a detailed description of the simulation, and finally, the LCA details.

\textbf{Case Studies.} The proposed case studies are defined from combinations of electricity and CO\textsubscript{2} sources, totaling eight different scenarios. CO\textsubscript{2} is captured from point sources at coal power plants (COAL, coal power plant capture scenario) or directly from the air (DAC, direct air capture scenario). Furthermore, H\textsubscript{2} is produced with a PEM electrolyzer. Water electrolysis can be powered by various energy sources, i.e., onshore wind (wind scenario), solar (solar scenario), nuclear (nuclear scenario), and grid electricity (current mix scenario). The rest of the FT plant (compressors, pumps) and the CO\textsubscript{2} capture processes consume energy from the current mix.
Global warming assessment breakdown of FT e-diesel synthesis based on different electricity and CO₂ sources. Comparison with fossil diesel production. The “other” category comprises the impacts of catalysts, natural gas heating, cooling, feed water, and electricity consumption at the plant (from the current mix). A further breakdown of the “other” category can be found in Figure S39. This figure is divided into two subfigures: the first one (left) comprises the case scenarios that combine DAC CO₂ and the four different electricity sources (wind, solar, nuclear, and current mix) for H₂ production, while the right one shows the same electricity scenarios but in combination with COAL CO₂ instead.

**e-Diesel Production Plant Simulation Overview.** We consider a simplified e-diesel process flowsheet, consisting of six different sections, as seen in Figure 2. H₂ and O₂ are produced in a PEM electrolyzer from water and electricity in the first section. The product H₂ and the unreacted water are mixed with CO₂ and enter a reverse water gas shift (RWGS) reactor where CO is generated. The mixture, which contains an H₂/CO ratio of two, enters the FT reactor, where diesel, gasoline, kerosene, light hydrocarbons, and waxes are synthesized. From here, heavy liquid waxes (C₁₅₋₂₁) and a fraction of the hydrogen from the first section are fed to the hydrocracking (HC) reactor, where waxes are broken down into more valuable hydrocarbons, mainly in the diesel fraction (C₁₄₋₂₀).

Both unreacted waxes and lighter paraffins join the main product stream of the FT reactor and enter the separation section, where the gaseous and aqueous phases are removed. The gaseous phase, mainly composed of unreacted H₂, CO, CO₂, and the C₁₋₄ fraction of the FT products, is sent to the furnace, where it is burned with part of the O₂ produced in the first section. The oxy-combustion produces a clean flue gas (CO₂/H₂O) from which CO₂ can be easily separated via water condensation and used to partially feed the RWGS reactor. The aqueous phase, which contains traces of dissolved CO₂, is modeled as wastewater. The organic phase, containing the C₅₋₁₂ fraction of the FT products, is sent to a separation train of three columns. In the first column, waxes (C₁₂₋₁₅) are separated from the fuels and sent to the HC reactor. In the second column, diesel (C₁₃₋₁₇) is recovered as the bottom product, and lastly, in the third column, the byproducts, gasoline (C₅₋₄) and kerosene (C₁₀₋₁₄) are separated. More details on the design as well as the simulation results can be found in Sections A and B in the Supporting Material.

**Life Cycle Assessment.** We carried out an LCA following the ISO 14040/44 framework.30 Regarding phase 1, the goal of the LCA is to compare the FT e-diesel to fossil diesel. The functional unit of choice is one kg of FT e-diesel. We adopted a cradle-to-gate scope following an attributional approach. The system boundaries cover all the upstream activities, from the synthesis of H₂ and CO₂ to diesel production. Co-production of kerosene and gasoline was modeled via system expansion with avoided burdens.

Concerning the inventory phase, we compute the life cycle inventory (LCI) of emissions, waste, and feedstock requirements by integrating information from the foreground and background systems. The foreground system was modeled by combining mass and energy flows from the process simulation implemented in Aspen HYSYS, complemented with literature sources for the CO₂ and H₂ feedstocks. The background system was modeled by using activities from Ecoinvent v3.5 (accessed via SimaPro v9.2.0.2).31

In the third phase of the LCA, the life cycle impact assessment (LCIA) was carried out to translate the LCI entries into the corresponding impacts following the ReCiPe 2016 v1.03.

**Total Annualized Cost.** The total annualized cost (TAC) was calculated as the sum of the annualized capital cost (AF-CAPEX) and the operating cost (OPEX) per year of plant operation (eq 1).

\[
TAC = AF - CAPEX + OPEX
\]  
(1)

where a 30-year time horizon and a 7% interest rate (IR) are considered.

Operating costs include the expenses of acquiring raw materials, consumption of electricity, and utilities. We compute the OPEX using eq 4.

\[
OPEX = OPEX^{\text{CO}_2} + OPEX^{\text{C}_\text{w}} + OPEX^{\text{Cl}} + OPEX^{\text{CH}_4} + OPEX^{\text{C}^C}
\]  
(4)

where \(OPEX^{\text{CO}_2}\) and \(OPEX^{\text{C}_\text{w}}\) are the total costs of CO₂ and water fed to the electrolyzer, respectively; \(OPEX^{\text{Cl}}\) is the total electricity cost used in the electrolyzer and the rest of the FT plant; \(OPEX^{\text{CH}_4}\) is the cost of heating; and \(OPEX^{\text{C}^C}\) is the cost of cooling. The prices of \(OPEX^{\text{CO}_2}\) electricity, and the electrolyzer, the most important contributors to the final cost, were retrieved from the literature. For CO₂ captured in a coal power plant, we use 39.5 $/ton (28–51 $/ton) based on pre-combustion capture with an integrated gasification combined cycle (IGCC) power plant,38 while for direct air-captured CO₂ we assume 200 $/ton (133–268 $/ton) as the mean value of low- and high-temperature capture plants working 8000 full load hours.34 For electricity, mean prices of 72.5 (44.3–100 $/MWh),35 139.5 (58.4–221 $/MWh),35 87.5 (62.8–112.2 $/MWh),36 and 94.3 $/MWh (44.3–144 $/MWh)37 are selected for wind, solar, nuclear, and the current mix, respectively. The cost of installing and operating the PEM electrolyzer was set at a conservative value of 850 $/kWh (400–1000 $/kWh),36,38 with an efficiency of 70% (60–80%) of the HHV.36,39,40 A more detailed explanation of the CAPEX and OPEX calculations and parameters can be found in Section E in the Supporting Material.
Externalities. Environmental impacts can be converted into monetary units using monetization factors. Notably, the three LCA endpoint impact categories (human health, ecosystem quality, and resource scarcity) can be translated into monetary units, known as externalities using suitable methods.\(^\text{41}\) The cost associated with the externalities (cost\(_{\text{EXT}}\)) is computed using eq 5:

\[
\text{cost}_{\text{EXT}} = \sum_e E_{\text{EI}} \cdot \text{MF}_e
\]

where \(E_{\text{EI}}\) is the in impact endpoint \(e\) and \(\text{MF}_e\) is the associated monetary factor. Based on the work by Freire-Ordoño, for human health, we consider a value of \(\text{MF}_{\text{HH}}\) of \(8.58 \times 10^4\) $/DALY, while for ecosystems quality, the monetary factor (\(\text{MF}_{\text{EQ}}\)) is \(1.10 \times 10^7\) $/species·year. Since resource scarcity is already measured in monetary units, we consider an \(\text{MF}_{\text{RS}}\) equal to 1.\(^\text{26}\)

Abatement Cost. The abatement cost is the tax that should be applied on CO\(_2\) for a carbon abatement technology to be able to match the cost of its fossil (business-as-usual, BAU) counterpart. We computed this metric using eq 6:\(^\text{42}\)

\[
\text{abatement cost} = \frac{C_{\text{new}} - C_{\text{old}}}{E_{\text{old}} - E_{\text{new}}}
\]

where \(C_{\text{new}}\) and \(E_{\text{new}}\) denote the cost and CO\(_2\)-eq emissions, respectively, of the new technology, more specifically, the TAC and global warming at the midpoint level for the different scenarios, and \(C_{\text{old}}\) and \(E_{\text{old}}\) (0.57 kg CO\(_2\)-eq/kg)\(^\text{43}\) represent the equivalent values for the substituted technology, in this case, fossil diesel. The production cost of fossil diesel was assumed to be 0.59 $/kg (0.4–0.6 $/L).\(^\text{24}\)

RESULTS AND DISCUSSION

The simulation results, including inlet and outlet flows and energy consumption, are reported in the Supporting Material (Section B). Additionally, 8.66 kg of O\(_2\) at 40 °C and 26.7 bar are produced per kg of diesel. This oxygen byproduct is excluded from the analyses since its potential commercialization depends on factors such as the location of the plant and the surrounding industries that may use it on-site.\(^\text{75}\) The LCA and economic results are discussed next.

Environmental Analysis Results. We report the midpoints and endpoints of the ReCiPe 2016 methodology. Out of the 18 midpoint categories, we focus on global warming, while the others are provided in the Supporting Material (Section C).

Figure 3 shows the global warming impact associated with the production of FT e-diesel. Overall, only two scenarios outperform fossil diesel, those based on DAC with wind and nuclear power, while the rest show higher carbon footprints. Notably, scenarios based on DAC CO\(_2\) outperform their COAL counterparts because CO\(_2\) is modeled as a negative flow (credit given for removing CO\(_2\) from the atmosphere). In the fossil case, CO\(_2\) is removed from the flue gases instead from the atmosphere, resulting in reduced emissions and lower carbon-intensive electricity (credit given to electricity generation; 1.13 kg CO\(_2\)-eq/kWh with no capture vs 0.29 kg CO\(_2\)-eq/kWh considering post-combustion capture). Furthermore, wind-DAC and nuclear-DAC scenarios lead to carbon-negative footprints. Among the

![Externalities](image-url)
remaining scenarios, COAL CO$_2$ scenarios relying on the current mix (43.5 kg CO$_2$-eq/kg) and solar (7.59 kg CO$_2$-eq/kg) perform much worse than the fossil analog (0.57 kg CO$_2$-eq/kg).

For both CO$_2$ sources, nuclear electricity can produce diesel with the lowest associated net impact (i.e., −3.87 kgCO$_2$-eq/kg diesel for DAC and 2.10 kgCO$_2$-eq/kg diesel for COAL) across all power sources. Wind electricity holds the second-best performance, when coupled with DAC, also reaching a negative net impact (−1.94 kgCO$_2$-eq/kg), followed by solar, and finally, the current mix. Notably, the current mix performs poorly because it is yet to be decarbonized (i.e., 0.54 kgCO$_2$-eq/kWh).

Concerning the impact breakdown, electrolytic H$_2$ emerges as the most significant contributor to the carbon footprint. This is followed by the CO$_2$ (in absolute value), then the gasoline byproduct, modeled as an environmental credit, the other category (i.e., electricity at the plant, heating, catalyst, and water usage), and the kerosene byproduct. Hence, low-carbon hydrogen is essential to produce low-carbon e-diesel, and so is the carbon source, which should be renewable (i.e., biogenic or from the air) to keep the carbon footprint of e-diesel low.

Figure 4 shows the endpoints for all of the scenarios. As seen, there is burden-shifting toward human health and, ecosystems quality, excluding the nuclear-DAC scenario. Notably, while two scenarios can reduce the carbon footprint relative to the fossil analog, none improves human health, and only nuclear-DAC can reduce the impact on ecosystems. In contrast, the resource scarcity category improves in all of the scenarios except the ones with the current mix. The trends are similar to those found in the carbon footprint analysis, i.e., nuclear performs best, followed by wind, solar, and current mix. Again, the current mix performs poorly, leading to extremely high impacts in all of the indicators.

Concerning the impact breakdown, again, electrolytic H$_2$ represents the main contributor, often followed by the other (plant electricity, catalyst, heating, and water usage) and CO$_2$ categories, and then the byproducts. The relative contribution of the other category is similar in human health and ecosystem quality for both CO$_2$ sources and is almost negligible in the resource scarcity indicator. Moreover, the CO$_2$ contribution of DAC also increases when shifting from human health to ecosystems, and also in resources, while it decreases in coal CO$_2$. Finally, the contribution of byproducts is low in human health and ecosystems in both CO$_2$ sources, however, increases sharply in resources. This is because byproducts are otherwise synthesized from oil, which is accounted for in resource scarcity. Hence, once again, it becomes clear that the hydrogen source dictates the overall environmental performance.

**Economic Results.** Figure 5 shows the results of the economic analysis considering the electricity costs reported in Section E in the Supporting Material (i.e., 0.072, 0.087, 0.094, and 0.139 $/kWh for wind, nuclear, the current mix, and solar, respectively). All the scenarios are more expensive than the business-as-usual, regardless of the electricity source. Wind attains the best performance, followed by nuclear, the current mix, and lastly, solar. The DAC scenarios are more expensive due to the higher cost of the captured CO$_2$ (0.20 $/kg vs 0.04 $/kg in the case of COAL).

Concerning the cost breakdown, OPEX clearly dominates CAPEX (75−85% in the DAC and 78−86% in the COAL scenarios). Note that electricity consumption, of which more than 99% is attributed to water splitting dominates the total cost, followed by the CO$_2$ source (10−16% in DAC and 2−3% in COAL) and other (including heating, cooling, and water fed to the electrolyzer), which barely reaches 1% of the total operating costs (0.6−1%). The cost of electrolytic H$_2$, computed as the sum of the costs of the electrolyzer and the electricity is 4.8, 5.8, 6.2, and 9.4 $/L diesel (7.9, 9.5, 10.3, and 15.5 $/kg H$_2$) for wind, nuclear, the current mix, and solar, respectively, representing a large percentage of the total cost across the scenarios (74−84% for the DAC and 86−91% for the COAL scenarios). These H$_2$ costs are in line with other reported costs of producing H$_2$ from renewable energy (4.6−10 $/kg H_2$ for wind, 4.99−8.21 $/kg H_2$ for nuclear, and 7.1−14.9 $/kg H_2$ for solar electricity). 36

The CAPEX, which makes up a significant percentage of the total cost (13−24% across scenarios), is dominated by the
electrolyzer (over 60%), followed by the reactors (33%) and other contributions (5%). Gasoline and kerosene loosely compensate for the capital costs of the plant. The contribution of selling these byproducts decreases the total cost of e-diesel, netting prices by 17–31% lower. In the scenarios of COAL, they also offset the cost of capturing CO₂.

Due to burden-shifting toward human health and ecosystems, the inclusion of externalities broadens the economic gap between fossil and e-diesel. The only exception is the DAC-nuclear scenario, with an associated externalities penalty of 0.07 $/L vs 0.61 $/L of fossil diesel. Notably, externalities are in the range 0.70–1.86 $/L (DAC) and 0.74–2.52 $/L (COAL), while the current mix scenarios lie above 11 $/L. Even though the externalities of the DAC scenarios are lower than those in their COAL counterparts (1.38 $/L vs 1.92 $/L for wind, 1.86 $/L vs 2.52 $/L for solar, and 0.07 $/L vs 0.74 $/L for nuclear, respectively), this difference is still insufficient to make DAC overall more economically appealing than COAL.

Finally, the abatement cost of the scenarios that lower the carbon footprint of fossil diesel amounts to 1520 and 2260 $/ton CO₂-eq in the wind and nuclear cases, respectively. This value exceeds by far the current estimated social cost of carbon emissions (60 $/ton CO₂-eq) as well as the most recent carbon market prices, i.e., 93.58 €/ton, 28.33 $/ton, and 56.00 $/ton, respectively, for the European Union, the United States, and Australia, to name a few.

**CONCLUSIONS**

In this work, we performed an environmental and economic analysis of Fischer–Tropsch electro-diesel using process simulation and LCA. E-diesel produced from nuclear-DAC can provide the best environmental results, while wind-COAL has the lowest cost.

The impact associated with the vast amounts of electricity consumed for water splitting, even if renewable, single-handedly surpasses fossil diesel’s global warming potential, also when accounting for avoided byproducts. Using renewable CO₂, i.e., from direct air capture, provides a net negative carbon source, and therefore, is mandatory to offset the impacts of H₂ production. This allows producing carbon-negative (on a cradle-to-gate) e-diesel (~1.94 kg CO₂-eq/kg diesel for wind and ~3.87 kg CO₂-eq/kg for nuclear). On the contrary, coal CO₂ does not reduce the carbon footprint of fossil diesel. However, e-diesel is still carbon-based. Consequently, the captured CO₂ would be released back to the atmosphere after combustion, making the overall life cycle (cradle-to-grave) still carbon positive.

All of the e-diesel alternatives, except nuclear-DAC, cause some collateral damage to human health and ecosystems, while improving resource scarcity. Burden-shifting is here due to the electrolytic H₂, which consumes massive amounts of renewable power. This behavior was also observed in biomass-based FT fuels, which raises concerns about whether synthetic fuels are the way forward in the quest for a fully sustainable transport sector.

The high costs of e-diesel, mainly linked to the electrolytic H₂, make it economically unappealing without carbon credits or other subsidies. However, the expected drop in the cost of renewables (i.e., 53–64% decrease in the 2009–2019 period for wind onshore), improvements in the electrolyzer, and cost reductions of the DAC technology (over 50% by 2030, and 3–4 times of current costs by 2050), combined with the rise of crude oil price, will help close the economic gap between the fossil and FT e-diesel, despite showing higher externalities.

Overall, FT e-diesel produced from wind or nuclear H₂ coupled with CO₂ from DAC could reduce the carbon footprint of fossil diesel substantially, yet they shift burdens to other environmental categories and, with the current state of technology, lead to prohibitive costs.

**ASSOCIATED CONTENT**

*Supporting Information*

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.2c01983.

Methodology and design of the simulation, life cycle inventory, further environmental results, and economic analysis (PDF)

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**Author Contributions**

The manuscript was written through the contributions of all authors. All authors have given approval to the final version of the manuscript.

**Notes**

The authors declare no competing financial interest.

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**ABBREVIATIONS**

BAU, business-as-usual; CEPCI, Chemical Engineering Plant Cost Index; COAL, coal power plant CO₂ capture scenario; DAC, direct air capture; e-diesel, electro-diesel; FT, Fischer–Tropsch; HC, hydrocracking; LCA, life cycle assessment; LCI, life cycle inventory; LCIA, life cycle impact assessment; PEM, proton exchange membrane; RWGS, reverse water gas shift; SOEC, solid oxide electrolyzer cell; TAC, total annualized cost

**NOMENCLATURE/ SUBSCRIPTS**

- **e** endpoint ∈ {human health, ecosystems quality, resource scarcity}
- **i** paraffin carbon number ∈ {1, 111}
PARAMETERS

- **$k$** process unit \( k \in \{ \text{compressor, pump, furnace, exchanger, tower, vessel, tray} \} \)

- **$A$** capacity [units depend on type of equipment]
- **$\bar{A}$** annualization factor \([y^{-1}]\)
- **$C_{\text{CO}_2}$** global average cost of selling fossil diesel \([\$/kg]\)
- **$E_{\text{CO}_2}$** global warming potential indicator of the production of fossil diesel \([\text{kg CO}_2\text{-eq/kg}]\)
- **$IR$** interest rate years
- **$M_{F_e}$** horizon time \([y]\)
- **$\alpha$** probability of propagation

VARIABLES

- **$C_{\text{mb}}$** bare module cost of process unit \( k \) \([\$]\)
- **$C_{\text{neq}}$** production cost of FT e-diesel \([\$/kg]\)
- **$C_{\text{CO}_2}$** cost of cooling \([\$/y]\)
- **$C_{\text{E}}$** cost of CO\(_2\) raw material \([\$/kg]\)
- **$C_{\text{e}}$** cost of electricity \([\$/y]\)
- **$C_{\text{H}}$** cost of heating \([\$/y]\)
- **$C_{P}$** purchased cost \([\$]\)
- **$C_{W}$** cost of water \([\$]\)
- **$\text{CAPEX}_{\text{EXT}}$** capital cost \([\$]\)
- **$\text{CAPEX}_{\text{new}}$** cost per kg of FT e-diesel \([\$/kg]\)
- **$\text{CAPEX}_{\text{EXT}}$** global warming potential indicator of production of FT e-diesel \([\text{kg CO}_2\text{-eq/kg}]\)
- **$E_{\text{FT}}$** impact of endpoint \( e \)
- **$n_{i}$** hydrogen stoichiometric coefficients in FT/HC reaction
- **$n_{i}$** paraffin of carbon number \( i \)
- **$\text{OPEX}$** operating cost \([\$/y]\)
- **$\text{TAC}$** total annual cost \([\$/y]\)

- **$\text{OPEX}$** operating cost \([\$/y]\)
- **$\text{TAC}$** total annual cost \([\$/y]\)
- **$\alpha$** molar fraction of paraffin with carbon number \( i \)

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