

Process Simulation, Integration and Energy Analysis of Direct Air Capture and Green Fischer–Tropsch Fuel Production

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Direct Air Capture (DAC) technology provides a promising way for extracting carbon dioxide (CO₂) directly from the atmosphere, enabling its use in either long-term sequestration or as a carbon source for synthetic green fuel production. In this study, CO₂ captured via DAC is combined with green hydrogen (H₂) to synthesize gasoline, targeting decarbonization of the transportation sector. To maximize system efficiency, a process integration strategy is employed. Tail gas and by-product oxygen from the electrolysis unit are recycled in the Allam cycle, a high-efficiency oxy-fuel combustion system, and in a Rankine cycle (RC) to generate electricity. The integration enhances both mass and energy utilization, boosting overall process performance. The process is modelled and integrated to evaluate its energy performance. Energy analysis of the green Fischer–Tropsch (FT) fuel pathway highlights the potential of DAC-based synthetic fuels as a solution for reducing CO₂ emissions.

1. Introduction

The production of green fuels using green hydrogen (H₂) and carbon dioxide (CO₂) presents a promising way for large-scale energy storage and CO₂ utilization, contributing to the decarbonization of hard-to-abate sectors (Uy et al., 2024). Among various synthetic fuel pathways, hydrocarbons (HCs) and gasoline synthesized via the Fischer–Tropsch (FT) process are particularly attractive as drop-in replacements for fossil-derived fuels (Schmidt et al., 2018). Notably, sustainable aviation fuel (SAF) derived from FT synthesis is poised to play a crucial role in reducing aviation-related CO₂ emissions due to its compatibility with existing infrastructure and aircraft engines. To support the transition to carbon-neutral fuel systems, techno-economic assessments of FT-based green fuel production have gained attention. For instance, König et al. (2015) modelled a power-to-liquid HC process and reported a process efficiency of 43.3 %. Zang et al. (2021) performed a comprehensive techno-economic analysis of FT fuel synthesis from CO₂ and H₂, emphasizing the importance of improving feedstock recycling and conversion ratios. More recently, Meurer et al. (2024) simulated a decentralized SAF production process optimized for kerosene yield, highlighting economic and operational trade-offs.

Despite these advances, existing studies often idealize the feedstocks—assuming pure CO₂ and H₂ feeds—and overlook the energy and integration challenges associated with upstream processes like direct air capture (DAC) and water electrolysis. In reality, these units, particularly when employing high-efficiency but endothermic technologies such as solid oxide electrolysis cells (SOECs), impose substantial thermal and electrical energy demands (Cinti et al., 2016). This can lead to overestimated efficiencies and misrepresented sustainability of the overall FT fuel production. To address these challenges, advanced energy integration strategies, such as the Allam cycle and Rankine cycle (RC), offer promising solutions. The Allam cycle, a novel oxy-fuel power cycle, can utilize purge gases and light hydrocarbons (HCs) from the FT process to generate CO₂-neutral, high-efficiency power with integrated CO₂ capture (Qi et al., 2025). Similarly, RC systems can recover low-grade waste heat from FT synthesis and upstream processes, converting it into electrical energy to offset the energy demands of DAC and SOEC units (Stempien et al., 2015).

This work investigates an integrated green FT fuel process based on DAC and SOEC technologies. The process is modelled to capture mass and energy balances across the process, with an emphasis on heat integration and resource utilization. Various configurations for utilizing purge gases and light HCs for internal energy recovery

are examined to improve overall process efficiency. This work offers an overview of the energy dynamics of the green FT fuel process, providing a basis for the development of more sustainable synthetic fuel pathways.

2. System description and model

2.1 System description

Figure 1 illustrates the diagram of the green FT fuel synthesis process. The overall process includes units such as DAC, SOEC, gas compression, and FT synthesis. Efficient heat integration and utilization of purge gas are essential to enhance process efficiency and lower fuel production costs. The following sections describe these three units to establish the basis for process design and integration.

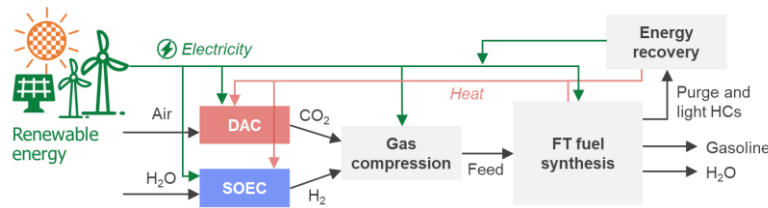


Figure 1: Concept of the green FT fuel process based on DAC and SOEC technologies.

2.1.1 SOEC

The SOEC is employed for its high efficiency and its potential for thermal integration with the FT synthesis reactor to utilize reaction heat. Designed to operate at high temperatures (700–900 °C), the SOEC can benefit from additional thermal energy recovery to reduce power consumption. The design of the heat exchanger network within the SOEC is critical for maximizing heat recovery and overall thermal efficiency. This work adopts the SOEC and its associated Balance of Plant (BoP) design from Liu et al. (2023). In this design, the high-temperature heating demand is fully recovered and self-sustained, leaving only low- to medium-temperature heating requirements, primarily for steam generation (around 100 °C).

2.1.2 DAC

The DAC captures CO₂ directly from air using an alkali-scrubbing-based approach, representing one of the most mature technologies. In DAC, CO₂ is absorbed in an air contactor using an aqueous KOH solution, forming K₂CO₃. The K₂CO₃ solution is then regenerated by reacting with calcium hydroxide to form calcium carbonate (CaCO₃), which is then fed into a calciner and decomposed into CaO and CO₂. Carbon Engineering pioneered this process, constructing a pilot plant and publishing detailed information (Keith et al., 2018). The design was later optimized to focus solely on capturing CO₂ from air (Sabatino et al., 2021). The primary energy demand of DAC arises from the regeneration, which relies on a calcium-based thermochemical cycle. High-temperature heat (~900 °C) for the calciner is supplied via oxy-combustion of methane, with oxygen produced through electrolysis. In this work, the DAC follows the minimal-energy design proposed by Sabatino et al. (2021).

2.1.3 Gas compression and FT fuel synthesis

The FT process is modelled based on the description by Fernández-Torres et al. (2022). In this configuration, H₂ and CO₂ are compressed to a high pressure of 3,000 kPa and fed into the synthesis section, which consists of two reactors in series. The first reactor facilitates the reverse water–gas shift (RWGS) reaction, converting CO₂ to CO, while the second carries out the FT synthesis to produce HCs. Following the reactions, a three-phase separator is used to separate water, gaseous products, and liquid HCs. Unconverted gases are recycled to improve overall conversion, while a purge stream removes excess H₂ to maintain system stability. Finally, a distillation column separates the HC products into light HCs and gasoline-range fuels.

2.2 Process simulation and integration

2.2.1 Simulation specifications

The commercial software Aspen HYSYS V14 is used to design and simulate the proposed green FT fuel process, which is shown in Figure 2. Simulations of the subunits are based on parameters from previous studies, as surmised in Table 1. The DAC simulation fully adopts the design proposed by Sabatino et al. (2021). The SOEC simulation builds on our previous work, where a grey-box model is employed using area-specific resistance derived from experimental data to calculate overvoltages (Qi et al., 2023). The cell voltage is calculated to be 1.293 V, with the SOEC operated slightly above its thermoneutral voltage, generating heat internally. Oxygen is

assumed as the sweep gas to aid in dissipating the heat produced within the SOEC. The reactor is simulated to accurately reproduce the product distribution observed in laboratory experiments, operating under isothermal conditions. In fact, two conversion reactors in series are used in simulation to simulate reverse water–gas shift (RWGS) and FT reactions reported by Fernández-Torres et al. (2022). To facilitate heat exchange within the FT synthesis unit, the FT reactor temperature is adjusted to be 10 °C higher than that of the RWGS reactor.

Table 1: Summary of key simulation parameters for the green FT fuel process.

Subunit	Parameter	Value	Subunit	Parameter	Value
SOEC	Current density / A/cm ²	0.70	DAC	Air velocity / m/s	0.5
	Temperature / °C	850		Calciner temperature / °C	900
	Area specific resistance / Ω/cm ²	0.47		Slaker temperature / °C	300
	Cell voltage / V	1.293		Capture rate / %	97
	Steam conversion rate	0.8		FT synthesis	RWGS temperature / °C
Gas compression	Compressor efficiency / %	75	FT temperature / °C		340
	Compression ratio	3.01	Reactor pressure / kPa		3,000
	Inter-stage cooling temperature / °C	40	H ₂ /CO ₂ feed ratio		3:1

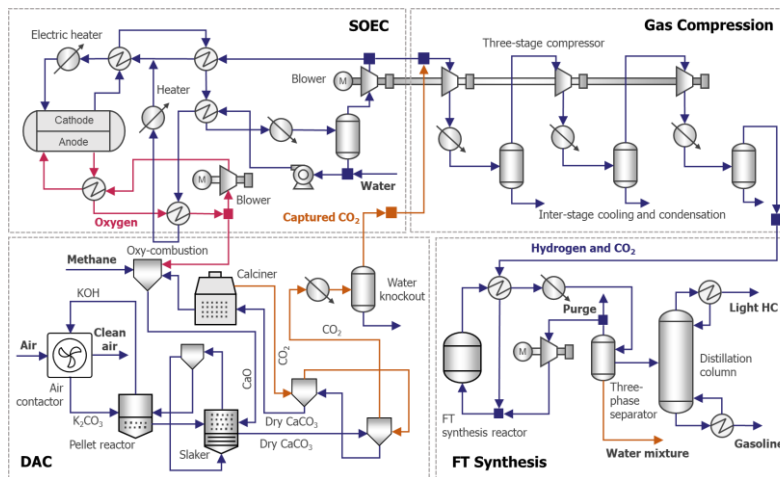


Figure 2: Diagram of the green FT fuel process.

3. Results and discussion

3.1 Base-case simulation results

The mass and heat balances for each unit are obtained through simulation. The energy requirements for each unit are summarized in Table 2, and an illustration of the entire process is provided in Figure 3. For the DAC, by utilizing the oxygen produced by the SOEC, the regeneration requires a significant amount of thermal energy (around 5 MJ/kg CO₂) compared to electricity consumption (0.38 MJ/kg CO₂). The oxygen generated by the SOEC is sufficient to meet the oxy-combustion needs. Gas compression also accounts for a notable share of electricity consumption. The heat from compression is not considered for utilization due to its low-grade nature. The SOEC exhibits a specific electricity consumption of 34.85 kW_e/kg H₂ and a specific heating demand of 5.162 kW_{th}/kg H₂. As a result, the reaction heat from FT synthesis can cover the SOEC heating demand.

Table 2: The energy and mass balances of each subunit (gas compression is abbreviated as 'comp').

Subunit	Parameter	Value	Subunit	Parameter	Value	
DAC	Specific heating demand / kW _{th} /kgCO ₂	1.389	Comp	Compressor power / kW _e	37,053.2	
	Specific electricity demand / kW _{th} /kgCO ₂	0.1056		FT synthesis	Recycle compressor power / kW _e	6,188
	Specific oxygen demand / kgO ₂ /kgCO ₂	0.3421			Reaction heat / kW _{th}	-83,252.6
SOEC	Specific electricity consumption / kW _e /kgH ₂	34.854	Distillation reboiler heat / kW _{th}	4,310		
	Specific heating demand / kW _{th} /kgH ₂	5.162	Purge + light HC flow / kg	14,431		
	Specific oxygen production / kgO ₂ / kW _e	0.22084	Gasoline flow / kg	23,653.4		

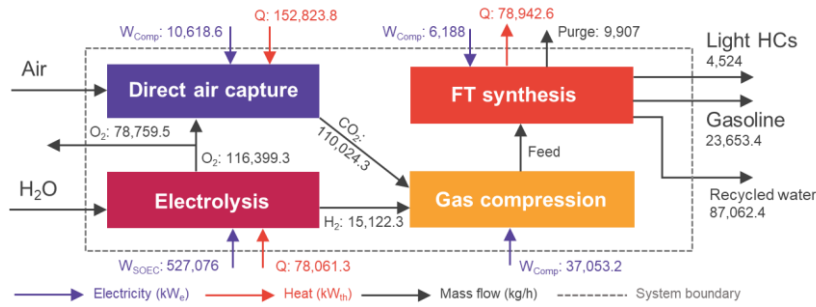


Figure 3: Mass and heat balances for the green FT fuel process.

3.2 Integration cases

In the process, the primary heat source is the reaction heat from FT synthesis, while the main heat sinks are the thermal energy required by the calciner—traditionally supplied by the oxy-combustion of methane—and the heat needed for steam generation in the SOEC. This work considers energy recovery strategies such as direct heat exchange between units and the utilization of purge gas for combustion to generate heat and power through the Allam cycle and the RC. Direct heat exchange between the SOEC and FT synthesis reactor is included, as the amount of heat generated exceeds the heating demand. Subsequently, the utilization of purge gas and light HCs for energy production becomes crucial to meet the energy needs of the DAC. Figure 4 presents four cases illustrating the use of purge and light HC gases for energy generation.

Case 1: Oxy-combustion for heating only

The purge gas and light HCs are directed to oxy-combustion solely for heating purposes. The generated heat is then supplied to the calciner to reduce external heat consumption.

Case 2: Oxy-combustion with RC for power generation

Building on oxy-combustion, the produced heat is utilized in a RC to generate power. The electricity produced offsets the overall power consumption of the process.

Case 3: Oxy-combustion with gas turbine for power generation

Instead of relying solely on the RC, a gas turbine based on combustion with air is employed for initial power generation. The remaining heat is then recovered and utilized by the RC to further enhance power output.

Case 4: Allam cycle for power generation

The purge gas and light HCs are directed into the Allam cycle to generate power efficiently.

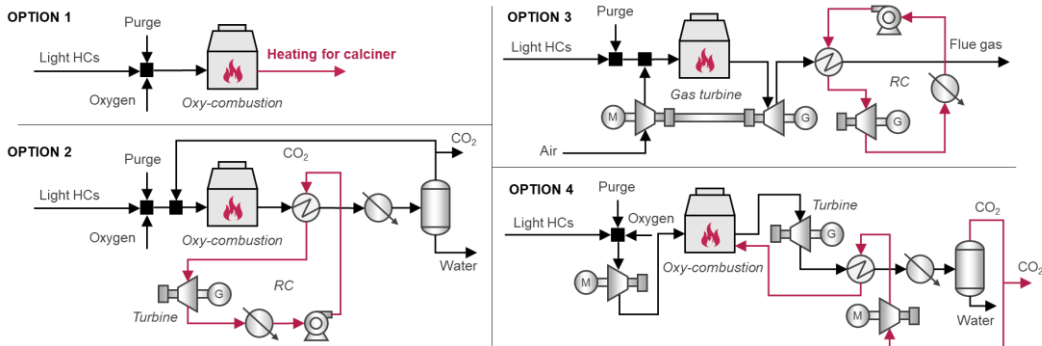


Figure 4: Four cases for utilization of purge and light HCs for heating and power generation.

3.3 Results and analysis

3.2.1 Energy generation result

Simulations of the four cases were conducted based on the presented process diagrams, and the resulting energy generation outputs are summarized in Table 3. In Case 1, the heating energy from oxy-combustion (132,840.3 kW_{th}) is insufficient to meet the calciner's energy demands. In Case 2, the RC generates 45,827.4 kW_e by utilizing this heating energy, assuming the flue gas is cooled to 150 °C. In Case 3, direct expansion of the flue gas produces 24,496.8 kW_e, with the remaining heat further used in the RC to yield an additional 24,301.8 kW_e. In Case 4, the Allam power cycle produces 114,837.3 kW_e—nearly double the output of Cases 2

and 3. Among the evaluated options, the Allam cycle demonstrates the highest efficiency for power generation from purge and HC gases.

Table 3: Energy generation results for 4 cases.

Case	Heating energy output (kW _{th})	Electrical energy output (kW _e)
Case 1	132,840.3	None
Case 2	None	45,827.4
Case 3	None	48,798.5
Case 4	None	114,837.3

3.2.2 Process energy integration

Figure 5 illustrates the heat and power integration of the green FT fuel process across four different cases. In all scenarios, the heat produced by FT synthesis is utilized within the SOEC, fully meeting its heating demand. In Case 1, despite utilizing heat from oxy-combustion, an additional 19,983.5 kW_{th} of external heating is still required. Although the CO₂ generated from oxy-combustion could be recycled back into FT synthesis—potentially affecting the overall heat balance—this aspect is not considered in the current analysis. In Case 2, the power generated is sufficient to meet the energy demands of both gas compression and FT synthesis. Case 3 yields slightly more power, enough to supply both the DAC and gas compression. However, Case 3 assumes the flue gas is not treated, which may require CO₂ to be captured together with ambient air in the DAC. This increases the heating requirement for DAC. Finally, in Case 4, the generated power is used to offset the electricity consumption of the SOEC, yet a deficit of 412,238.7 kW_e remains and must be supplied externally.

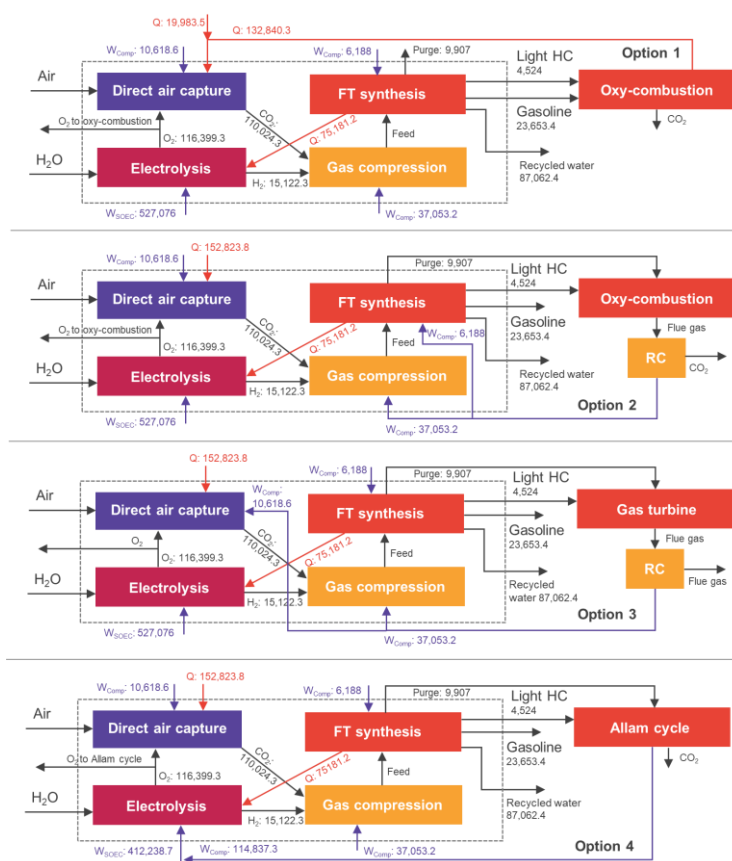


Figure 5: Heat/power integration for the green FT fuel process based on 4 cases.

3.2.3 Energy efficiency

Energy efficiency serves as a key indicator of process competitiveness. It is calculated using the usable energy content of the product stream, derived from the product mass flow rate (\dot{m}) and its lower heating value (LHV).

The total energy demand includes electrical power (P) consumed by the DAC, SOEC, and compressors in the gas compression and FT synthesis units, along with the heating energy (E_{fuel}) required by the DAC. The energy efficiency (η) is defined as Eq(1) (Tang et al., 2024):

$$\eta = \frac{\dot{m}_{Product} LHV_{Product}}{P_{DAC} + P_{SOEC} + P_{comp} + E_{fuel}} \quad (1)$$

The calculated energy efficiencies for the four cases are 47.45 %, 41.30 %, 41.56 %, and 46.07 %. Case 1 demonstrates the highest efficiency due to direct heating from oxy-combustion. Case 4 follows, assuming power is recovered from purge and HC gases. Across all cases, process efficiency ranges from 40 % to 50 %, indicating that further improvements are necessary to enhance overall energy performance.

4. Conclusions

This study presents an integrated simulation and energy analysis of green FT fuel production using CO₂ from DAC and H₂ from SOEC. Key integration strategies include direct heat exchange between the exothermic FT synthesis reactor and the SOEC, which effectively meets the SOEC's high-temperature heating demand and improves overall thermal efficiency. Additionally, purge and light hydrocarbon gases are utilized through various energy recovery systems—oxy-combustion, RC, gas turbines, and the Allam Cycle. Among the four cases, the Allam cycle (Case 4) achieved the highest power output, while direct oxy-combustion (Case 1) delivered the highest energy efficiency at 47.45 %. However, all scenarios required external energy inputs, indicating further optimization potential. This work demonstrates the value of full-process heat and power integration for enhancing the efficiency of DAC-based FT fuel production, offering a foundation for future improvements.

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