TECHNO-ECONOMIC ANALYSIS OF CARBON MITIGATION TECHNOLOGIES

CA21127

WG2 TrANsMIT Symposium on

Modelling approaches for CCUS

19 June 2026, online

Proceedings

DELIVERING HARMONISED
CCUS ASSESSMENT

PROCESS MODELING
TECHNO-ECONOMICS
LIFE CYCLE ASSESSMENT

Abstracts

Symposium program (CEST, UTC+2)

9:30 – 9:40	**P. Lisbona, M. Bailera** (WG2 Leaders). Welcome
9:40 – 10:00	**C. González-Fernández.** Multiphysics Modelling of CO_2 Electroreduction to Formate as a Digital Tool for Carbon Utilization.
10:00 – 10:20	**C. Barón.** Techno-economic assessment of the sorption enhanced methanation: Levelized cost of methane, performance indicators and sensitivity analysis.
10:20 – 10:40	**A. Al-Dafaie.** Allam Cycle Modeling Utilizing CoolProp and Excel.
10:40 – 11:00	**J. Roberto F.S.** Techno-Economic Analysis of Forest-Based e-Fuel Production Process Pathways.
11:00 – 11:20	**T. Gholizadeh.** Techno-economic and life cycle assessment of integrated SOEC and Fischer–Tropsch systems for synthetic fuel production from sewage sludge.
11:20 – 11:40	**I. Arnaiz.** First Principles Life Cycle Assessment of Sustainable Aviation Fuel via Methanol to Jet with Experimental Methanol to Olefins Data Integration.
11:40 – 12:00	**K. Quintana.** Can CO_2 Selective Membranes Improve the Techno Economic Performance of Fischer–Tropsch Synthesis?

Preface

Proceedings of Working Group 2 TRANSMIT Symposium on Modelling Approaches for CCUS

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Keywords: CCUS, Process modelling, validation, early-stage researchers, COST Action, TRANSMIT.

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It is our great pleasure to welcome you to the Proceedings of the Working Group 2 TRANSMIT Symposium on Modelling Approaches for CCUS, held online on June 19, 2026. This symposium serves as a pivotal forum under the framework of the COST Action CA21127 (TRANSMIT)—*Techno-economic analysis of carbon mitigation technologies*—bringing together researchers, engineers, and scientists dedicated to accelerating the deployment of Carbon Capture, Utilization, and Storage (CCUS) value chains.

The core thematic focus of this event centers on advanced process modeling of carbon mitigation pathways. In an era where the European chemical and energy sectors must urgently transition away from fossil feedstocks, rigorous mathematical and digital tools are vital to de-risk new technologies before industrial scale-up. In this context, this symposium places a special, dedicated emphasis on modeling approaches that have been tightly integrated with and validated by experimental data. Grounding simulation frameworks in real-world, laboratory, or pilot-scale evidence is paramount to ensuring the accuracy, reliability, and ultimate operability of future low-carbon infrastructures.

Crucially, this symposium has been deliberately designed and oriented as a specialized platform for PhD students and early-career researchers. Our goal is to provide a nurturing yet scientifically rigorous environment where doctoral candidates can present their ongoing research, stress-test their models against peer scrutiny, and engage in meaningful technical discussions with senior experts. The high quality and ambition of the abstracts compiled in this volume reflect the vital role that the next generation of researchers plays in delivering harmonized, replication-ready CCUS solutions.

Finally, we would like to express our deepest gratitude to the COST Action TRANSMIT and the European Cooperation in Science and Technology. Their support, funding, and networking framework have been instrumental in fostering this cross-border collaboration and making this event a reality. We also extend our sincere thanks to the peer reviewers for their invaluable time, and, above all, the authors and doctoral students whose groundbreaking contributions drive the success of this symposium.

We trust that these proceedings will provide you with valuable insights and inspire further innovations in the field of carbon mitigation.

Prof. Manuel Bailera, Symposium Organizer / WG2 leader
Prof. Pilar Lisbona, Symposium Organizer / WG2 co-leader

WG2 TrANsMIT Symposium on Modelling approaches for CCUS (19th June 2026)

Multiphysics Modelling of CO_2 Electroreduction to Formate as a Digital Tool for Carbon Utilization

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Abstract

This study focuses on the development of a three-dimensional multiphysics model for the electrochemical conversion of CO_2 ($ERCO_2$) to formate, providing mechanistic insight into cell performance and guiding the design of CO_2 electrolyzers. The study focuses on the cathodic compartment of a gas diffusion electrode (GDE)-based electrolyzer and is carried out in COMSOL Multiphysics 6.2. The model is first validated against experimental data, and subsequently used to systematically investigate the system performance under conditions relevant to post-capture streams by varying the inlet CO_2 concentration within the range 40-100% (v/v). The model enables the identification of the operating regimes where $ERCO_2$ and the undesired hydrogen evolution reaction (HER) compete, while also resolving spatially varying concentration profiles inside the electrolyzer. Overall, the results highlight the importance of multiphysics simulations for modelling CO_2 electrolyzers and demonstrate the potential of the model as a predictive tool to guide system design.

Keywords: CO_2 electroreduction; *Formate*; *GDE*; *Multiphysics model*; *Operating regimes*.

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1. Introduction

Electrochemical conversion of CO_2 ($ERCO_2$) to valuable chemicals and fuels has emerged as a promising pathway for carbon utilization. Special attention has been devoted to $ERCO_2$ to formate ($HCOO^-$) due to the industrial relevance of this product. [1, 2] Therefore, important advances have been made in $ERCO_2$ to $HCOO^-$ through progress in reactor configuration, electrode structure, and operating conditions. [2,3] In this context, gas diffusion electrode (GDE)-based electrolyzers have demonstrated enhanced CO_2 accessibility to the catalyst surface, thus promoting the electrochemical process. However, their performance is governed by a complex interplay of different phenomena, namely, electrochemical kinetics, mass transport, homogeneous reactions and fluid flow, which has been primarily investigated experimentally. [1,2] Gaining an in-depth understanding of these coupled phenomena under industrially relevant conditions (i.e., high current densities or diluted CO_2 feed streams) remains challenging using experiments alone. [1,4,5] In this regard, multiphysics simulations represent a powerful tool to provide insight into the governing phenomena, thus complementing experimental evidence and guiding the design of efficient electrolyzers. While several one- and two-dimensional models have been already developed, they typically rely on simplifying assumptions that limit their ability to accurately capture the system performance under conditions relevant to industrial operation, where spatial heterogeneities become important. [3-7] To contribute to addressing this research gap, a three-dimensional (3D) model for $ERCO_2$ to $HCOO^-$ is herein developed. The model enables the investigation of realistic operating conditions, including variations in inlet CO_2 concentration, and allows identification of operating regimens based on the competition of $ERCO_2$ and the undesired hydrogen evolution reaction (HER).

2. Methods

This study focuses on the cathodic compartment of a GDE electrolyzer, which derives from the work of Díaz-Sainz et al. [1] In particular, our model explicitly comprises four distinct domains, namely: gas and catholyte channels, gas diffusion layer (GDL) and catalyst layer (CL). The $ERCO_2$ and the competing HER take place in the CL, yielding the desired $HCOO^-$ (eq. 1) and H_2 (eq. 2), respectively:

$$\mathrm{CO_2 + 2e^- \rightarrow HCOO^- + OH^-\ (E_0 = -0.02\ vs.\,RHE)} \quad (1)$$

$$\mathrm{2H^+ + 2e^- \rightarrow H_2\ (E_0 = 0\ V\ vs.\,RHE)} \quad (2)$$

Briefly, the model accounts for: [3-7]

- Mass, momentum, and ion transport within the GDL, CL and gas and catholyte channels
- Phase transfer of gaseous CO_2 into the liquid electrolyte at the GDL-CL interface
- Electrochemical kinetics modeled through concentration-dependent ($ERCO_2$) and concentration-independent (HER) Butler-Volmer equations
- Homogeneous reactions

The model is solved at steady-state in COMSOL Multiphysics 6.2 and is used to investigate the effect of feed composition (CO_2/N_2 mixture) on the system performance. In particular, it comprises the following physics interfaces: "Secondary current distribution", "Transport of concentrated species", "Transport of diluted species", and "Free and porous media flow, Brinkman". A physics-controlled mesh, which contains 13091 domain, 9804 boundary and 1444 edge elements, is defined. The model is computed through a segregated approach using MUMPS solver.

3. Results and discussion

First, the reliability of the model for reproducing the system performance is assessed by comparing the Faradaic efficiency toward $HCOO^-$ (FE_{HCOO^-}) obtained from simulations and experiments (Figure 1). Simulation results exhibit good agreement with experimental data across the entire range of tested feed compositions, demonstrating the accuracy of our model.

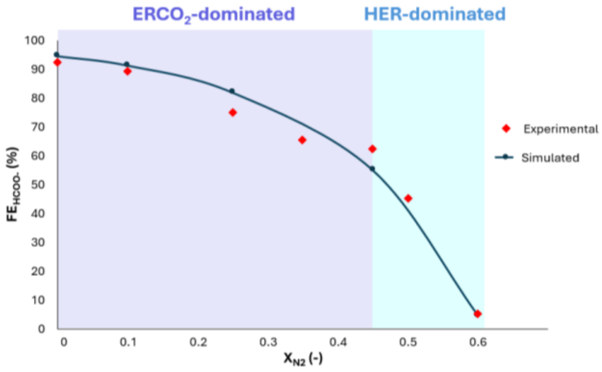

Figure 1. Faradaic efficiency as a function of inlet composition (CO_2/N_2 mixture).

Once the model is validated, it is used to gain insights into the two operating regimens that can be recognized from Figure 1. In particular, for N_2 mole fractions in the feed below 0.45, $ERCO_2$ dominates over HER, resulting in FE_{HCOO^-} higher than 55%. Conversely, for high N_2 mole fractions (>0.45), HER becomes the dominant reaction, leading to a significant drop in FE_{HCOO^-}, which reaches negligible values at N_2 mole fractions around 0.6. The CO_2 distribution profiles predicted by the simulations (Figure 2) reveal that this performance is caused by the reduction in overall availability of CO_2 in the electrode due to its dilution in the inlet stream. Hence, a CO_2 mole fraction in the feed of ~0.55 represents a critical threshold since lower concentrations entail a shift of product selectivity from the target $HCOO^-$ to H_2.

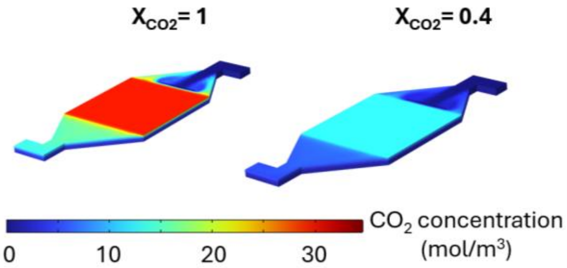

Figure 2. Distribution of CO_2 concentration in the electrode for different CO_2 partial pressures in the feed stream.

4. Conclusions

This study presents a 3D model for $ERCO_2$ to $HCOO^-$ in the cathodic compartment of a GDE electrolyzer. The model accurately reproduces experimental measurements of FE_{HCOO^-}. Additionally, it allows for gaining insights into the species distribution inside the electrolyzer that causes the shift between $ERCO_2$ to HER-dominated regimens when the N_2 mole fraction in the feed is increased. Overall, the results highlight the importance of multiphysics simulations for modelling CO_2 electrolyzers and demonstrate the potential of the model as a predictive tool to guide system design.

Acknowledgements

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Techno-economic assessment of the sorption enhanced methanation: Levelized cost of methane, performance indicators and sensitivity analysis

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Abstract

This work presents the first techno-economic assessment of sorption-enhanced methanation (SEM, TRL-3) using experimental data, compared with conventional methanation (CM). Experimental results supported a kinetic model for reactor sizing. CM requires 70–90 kg of catalyst per MW_e of electrolyzer, whereas SEM requires 223.7 kg/MW_e. For a 200 MW_e plant, both technologies show similar CAPEX (~500 M€), but SEM generates up to three times higher revenues due to the higher methane purity achieved. CM is economically unviable at 95% CH_4 purity, with a levelized cost of methane (LCOM) of 2.4–3.3 €/kg, exceeding natural gas market prices. At 99% purity, CM may become marginally profitable. SEM shows a comparable LCOM (~3.5 €/kg_{SNG}) but can target the premium 99.9% CH_4 market (~12 €/kgCH_4), ensuring profitability even under unfavorable hydrogen costs. SEM could therefore support the maturation of innovative hydrogen production technologies.

Keywords: Sorption-enhanced methanation; levelized-cost; techno-economic assessment; industrial decarbonization

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1. Introduction

Carbon dioxide (CO_2) is a primary driver of global climate change, and with a growing world population and the accelerating industrialization of developing nations, immediate and effective strategies are essential to limit its impact. In this context, CO_2 utilization has gained significant attention as a promising approach, enabling the conversion of these CO_2 emissions into valuable fuels and chemicals, thereby mitigating resource depletion.

The power-to-methane (PtM) process involves producing hydrogen via water electrolysis using surplus renewable electricity, which is then reacted with captured CO_2 to generate synthetic methane through the Sabatier reaction (eq. (1)).

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O \tag{1}$$

Nevertheless, over the past decade, an alternative process intensification strategy has emerged as a promising approach to moving beyond conventional methanation (CM). This approach, known as Sorption-Enhanced Methanation (SEM), integrates the reaction and separation processes in a single step, offering new opportunities to overcome the thermodynamic and kinetic limitations inherent in traditional systems.

The SEM process combines CO_2 methanation with in-situ H_2O removal by incorporating a solid sorbent into the reactor. According to Le Chatelier's principle, the continuous adsorption of the formed H_2O shifts the equilibrium towards CH_4 production. This results in higher conversions and methane yields under milder operating conditions. This work presents the techno-economic assessment of the SEM process. The simulations are based on experimental data obtained under different operating conditions and are benchmarked against CM. Moreover, it is the first study to provide the levelized cost of methane for SEM processes.

2. Methods

Both CM and SEM will be modelled in Aspen Plus v.11 based on experimental data, obtained at a lab-scale TRL-3 reactor. In both cases, the same commercial Nickel-based catalyst is used, supplied by Haldor Topsoe. For the SEM process, the chosen adsorbent is a commercial zeolite 4A supplied by Thermoscientific. The TRL-3 reactor has been described in previous publications by the authors. Afterwards, valuable insights such as the mass of catalyst needed, the case-specific thermal integration performed, and the economic revenue will be extracted.

From the technical side, in all cases a mixture of 60 vol.% CO and 40 vol.% CO_2 is converted into CH4 by using the corresponding stoichiometric amount of H_2. For the conventional methanation process, purities of 95% and 99% will be obtained, whereas for SEM it is 100% (assumed 99.99%). For comparison purposes, a 1 MW_e PEM electrolyzer was considered (4.4 kWh/Nm^3 consumption, producing 20.4 kg/h of hydrogen). No impurities were considered.

The economic analysis was assumed to be a retrofit of an existing industrial plant who desired to abate their emissions, revalorizing them. CAPEX, OPEX and incomes were calculated under a 20-year time framework, and the levelized cost of methane that rendered profitability (NPV = 0) calculated.

2.1. SEM

The SEM is based on the operation of a reactor filled with both catalyst and adsorbent, alternating methanation and regeneration stages. In the methanation stage, the adsorbent traps the water produced during methanation, shifting the equilibrium towards CH_4 formation. During the regeneration phase, water is desorbed. A continuous SNG stream can be obtained when several reactors operating in parallel are considered. When one reactor is performing methanation, the others are desorbing water. For this case study, a setup with four reactors is considered, where methanation and regeneration take 15 and 45 minutes. The methanation reactor operates at 10 bar and 240 ºC under stoichiometric $H_2/CO/CO_2$ feed gas conditions. Outlet purity is 100% assumed 99.99%).

2.2. CM

In conventional methanation, the reactor is filled with silicon carbide (CSi) and catalyst in a mass ratio of 4 to resemble the SEM arrangement. The gaseous feed stream is compressed just to overcome the pressure losses downstream. Depending on the configuration, a train composed of a heater, a fixed-bed reactor and a condenser is repeated a different number of times The target is to either reach a grid-quality SNG (95 vol.% CH_4) or an industrial-grade SNG (99 vol.% CH_4), while keeping at minimum the amount of catalyst used through a kinetic model derived from the CM experiments. Different configurations are considered, varying the amount of reactors (2, 3 or 4), the presence or not of technical constraints (maximum GHSV, minimum temperature of operation), pressure (1 or 10 bar), and the desired purity (95 or 99%).

3. Results and discussion

Experimental results demonstrate that CM presents the three characteristic operating regimes: (i) low temperature, (ii) intermediate temperature but high GHSV, and (iii) optimal temperature with moderate-to-low GHSV. Conversions above 90% required low temperature (under 250 ºC) and low GHSVs. Contrarily, SEM conditions resulted in CH_4 purity of up to 100 vol.%, due to the *in-situ* adsorption of H_2O by the zeolite, bypassing the thermodynamic limitations under those conditions (95.8 vol% d.b CH_4).

Aspen Plus simulations proved that, for the CM cases, best results (less catalyst and electricity consumption, and better heat integration) were obtained with 4 reactors for 95% CH_4. However, once technical constraints were considered, 3 reactors were the best and only realistic choice. For 99% CH_4, pressurization to 10 bar was necessary, as otherwise it is not realistic to achieve 99% (over 13 reactors needed) In all cases, most of the heating was covered by heat integrations, assessed through a Pinch analysis. The total cooling demand was similar in all cases, as it is related to the reaction itself (170 kW/MW_e). The SEM cases present the highest catalyst consumption (223.7 vs. 70–90 kg/MW_e), as it uses 4 reactors in parallel. All cases present a LCOM of around 2.4- 3.9 €/kg_{SNG}. However, they access different markets (95% SNG is sold at 0.5 €/kg, 99% at 4.2 €/kg, and 100% at 12 €/kg).

4. Conclusions

This paper presents a techno-economic comparison of different conventional methanation (CM) and sorption enhanced methanation (SEM) schemes. Both are supported by experimental data. Results show that it is not realistic for CM to go over 99% purities due to thermodynamic limitations. That limitation is overcome by SEM due to in-situ water absorption. As a result, SEM presents access to a 99.99% purity premium market that presents a great range of profitability. Contrarily, CM schemes with 99% are only marginally profitable, whereas 95% purities are not fit for the market. SEM could therefore support the maturation of innovative hydrogen production technologies.

Acknowledgements

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Allam Cycle Modeling Utilizing CoolProp and Excel

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Abstract

This study presented an Excel-based, steady-state, first-law thermodynamic model of the supercritical carbon dioxide (sCO_2) Allam cycle. To address ideal gas limitations in supercritical regimes, the CoolProp library was integrated to precisely calculate sCO_2 enthalpies. The methodology defines an oxy-combustor operating with pure methane, a multi-stage compression network, and a discrete Air Separation Unit that modeled air as an ideal binary mixture to iteratively calculate a polytropic index matching a specific power target. The 6-stage turbine employed continuous adiabatic mixing to simulate blade cooling, discharging into an isentropic subsonic diffuser for exhaust recovery. Crucially, the recuperator was integrated with the main air and CO_2 compressors, capturing intercooler rejected heat to preheat the high-pressure recycle and oxygen streams. Validated against benchmark data, the model predicted net plant output and efficiency with accuracy of 4.3% and 2.7% versus IEAGHG report data, respectively, offering a simplified, in-house framework for component-level thermodynamic evaluation.

Keywords: Allam Cycle; *CoolProp*; *Air Separation Unit*; *Carbon Capture*; *Supercritical CO_2.*

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1. Introduction

Modeling the Allam Cycle using commercial software presents challenges due to the lack of experimental data [1]. Previous literature utilized commercial software such as Aspen Plus and EES, though frequently with simplified turbine and ASU modeling approach [2], [3]. This droves the concept of developing an in-house simulation tool utilizing Excel and CoolProp [4]. The tool was built to model Allam Cycle at the component level using first and second laws of thermodynamics.

2. Methods

2.1. Boundary Conditions and Fluid Properties

The plant is modeled at standard ISO conditions (15°C, 1.013 bara, 60% relative humidity). A 100% methane (CH_4) fuel stream is supplied at 70 bara to enable exact stoichiometric calculations of oxygen demand and the subsequent tracking of pure CO_2 and H_2O generation. Air is defined as a binary mixture of 77% N_2 and 23% O_2 by weight, with an adjusted molecular weight of 28.16 kg/kmol to account for the argon component [5]. Because the Allam cycle operates extensively in the supercritical region of CO_2, where ideal gas assumptions are strictly invalid, the CoolProp [4] library is utilized to estimate accurate supercritical CO_2 enthalpies. Constant specific heat assumptions are applied only where temperature differences between states justify such a simplification. The Allam cycle is also modeled under pure CO_2 assumption.

2.2. Component-Level Assumptions

Compressors: Fuel and CO_2 compression are modeled using multi-stage isentropic compressors with interstage cooling. Air compression utilizes polytropic compressors. The design assumes centrifugal compressors with a maximum pressure ratio of 4.5 per stage [6]. The CO_2 main compressor output is mechanically coupled [7] to the turbine and set to 80 bara [8], after which the flow is condensed and pumped to final pressure.

Air Separation Unit (ASU): Air is compressed to ~120 bara [9] then it undergoes a perfect separation process modeled for a two-component ideal gas mixture [10]. The system is constrained by a target specific power consumption of 0.357 kWh per kg of 99.9% pure O_2 produced [11]. Within the Excel framework, a solver routine iteratively adjusts the assumed polytropic index of the compression process until the calculated ASU specific work matches this specific power constraint. Finally, the generated oxygen stream undergoes secondary compression to meet the required operating pressure of the oxy-combustor.

Combustor: Modeled for complete combustion of pure O_2 and 100% CH_4 that produces heat, CO_2, and H_2O. The combustion mixture is adiabatically mixed with recycled CO_2 to achieve a fixed turbine inlet temperature of 1150 °C [12].

Turbine: High temperature sCO_2 expands across 6 stages with an estimated overall efficiency of 92%; the turbine cooling flow is set to 8% of total exhaust flow [7]. Bocher et al. [13] work has been utilized to obtain the stage temperatures that were applied in designing the turbine. The model assumes adiabatic mixing between the mainstream and coolant flows at each stage to represent blade cooling effects. The coolant temperature is assumed to be the weighted average of the main flow and cooling flow temperatures. Turbine design approach is shown in Fig. 1. The exhaust is processed through a subsonic isentropic diffuser to recover pressure and temperature [10].

Recuperator: Modeled as a control volume using an overall energy balance. Also, the recuperator is thermally integrated with CO_2 and air compressors to capture the energy from the intercooling process. It also heats the oxygen and converts it from liquid to gaseous state.

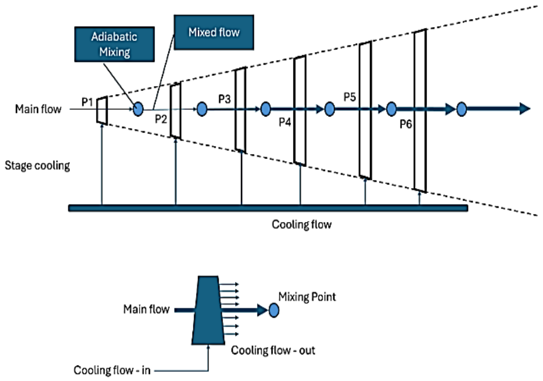

Figure 1. Turbine design approach

2.3. Modeling methodology

The model is built under similar boundary conditions found in Allam et al. [8] and IEAGHG [12]. The energy input, combustion coolant temperature, turbine inlet temperature and pressure, turbine stages temperatures, and turbine exhaust temperature were considered constraints for the model. The model is iteratively solved to achieve energy and mass balance using Macro-based Excel goal-seek function. In addition, the recuperator was tuned under fixed turbine exhaust and oxygen flows exit temperatures.

3. Results and discussion

The accuracy of the developed excel-based thermodynamic tool is evaluated by comparing its outputs against established IEAGHG report [9]. The tool accurately estimated the combustor exit flow with -2% accuracy, turbine exhaust flow with -5.1% accuracy, air flow with -3.3% accuracy, and O_2 flow with -0.1% accuracy. Concerning the performance, the gross output accuracy is 8.2%, total main systems (CO_2 compressor, ASU, and gas compressor) power consumption accuracy was 0.9%. The net power output and efficiency had accuracy of 4.3% and 2.7% respectively. The plant auxiliary loads assumed equal to the reported values in IEAGHG [12]. Table 1 shows this work results versus IEAGHG data. In addition, incorporating the diffuser enabled to estimate the turbine exhaust pressure with a higher accuracy compared to the IEAGHG value. Allam et al. [8] reported an exhaust pressure of 30 bara, which the tool was able to estimate. In fact, the estimated pressure ratios across the different stages were estimated with less than ±2% accuracy. The total exhaust mass flow is different as the turbine cooling flow basis is different. It is taken as 8% of the total flow [7]. The turbine cooling temperature is estimated based on the overall energy balance.

Table 1. This work results versus IEAGHG

Mass, T and P	This work	IEAGHG [12]	Performance	This Work	IEAGHG [12]
Gas from combustor	4,461,045	4,552,820 kg/h	Turbine gross output-electr.	1,155.2 MW	1068 MW
Turbine cooling flow	387,916 kg/h	521,750 kg/h	CO_2 compress. work	217.7 MW	197.9 MW
Turbine cooling temp	478 °C	400 °C	ASU	154.8 MW	170.7 MW
Total turbine exhaust flow	4,848,961 kg/h	5,074,570 kg/h	Gas compress. load	8.0 MW	8.6 MW
Air flow	961,221 kg/h	994,250 kg/h	Tot. aux. power consum.	380.5 MW	377.2 MW
Turbine exhaust press	30 bara	34 bara	Utilities aux load	29 MW	29 MW
Turbine exhaust temp	775 °C	740 °C	Plant net output	891.5 MW	854.4 MW
Oxygen flow	221,081 kg/h	221,390 kg/h	Plant net efficiency	58.05%	55.40%

4. Conclusions

A steady-state first-law thermodynamic model of the Allam cycle was developed. The integration of the CoolProp library resolved supercritical CO_2 enthalpies, supporting the explicit mathematical modeling of the ASU, multi-stage compression, and a 6-stage cooled turbine. The model accurately estimated the net output and efficiency within less than 5% error, validating the applied component-level methodologies against established IEAGHG data. This structured mathematical framework provides a basis for evaluating specific cycle parameters and component interactions.

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WG2 TrANsMIT Symposium on Modelling approaches for CCUS (19th June 2026)

Techno-Economic Analysis of Forest-Based e-Fuel Production Process Pathways

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Abstract
This work presents a techno-economic assessment of a decentralized Power-to-Fuel platform using forest management residues as a biogenic CO_2 source for methane, methanol, sustainable aviation fuel, and diesel production. A unified system boundary was adopted, including biomass pre-treatment, combustion-based cogeneration, flue gas cleaning, cryogenic CO_2 capture, PEM electrolysis, and fuel-specific synthesis and upgrading. Simulations were performed in MatLab for a fixed biomass throughput of 200 kt/y of FMR (550 GWh/y), while economic performance was assessed through unit production cost, levelized cost of fuel, sensitivity analysis, and scale effects. Results show that electrolysis dominates system electricity demand (>91%), making hydrogen production the primary cost driver. Methanol is the most competitive option on a mass basis (0.99 €/kg), whereas methane becomes preferable on an energy basis (154 €/MWh). The results indicate that competitiveness depends mainly on electricity price and electrolyzer efficiency improvements.

Keywords: e-Fuels; *Forest residues*; *Anti-sublimation*; *Carbon capture*; *Techno-economic analysis*.

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1. Introduction

Renewable e-fuels produced from captured CO_2 and green H_2 are increasingly recognized as key options for decarbonizing hard-to-abate sectors, including aviation, maritime transport, and heavy-duty industry, where direct electrification remains challenging [1]. When biogenic CO_2 is employed as the carbon source, Power-to-Fuel (PtF) pathways can contribute to near-closed carbon cycles while simultaneously supporting renewable energy integration [2]. In this context, Forest Management Residues (FMR) represent an attractive feedstock due to their local availability, wildfire mitigation role, and potential for sustainable fuel and forest management.

Several techno-economic studies have evaluated methane, methanol, and Fischer-Tropsch (FT)-based fuel pathways. However, most focus on single-fuel systems and centralized plants [3]. Comparative assessments using a common biomass-derived CO_2 platform and cryogenic capture remain limited. Therefore, this work develops a harmonized techno-economic framework to compare methane, methanol, Sustainable Aviation Fuel (SAF), and diesel production from forest-based biogenic CO_2.

2. Methods

A decentralized PtF system shown in Figure 1 was modelled in MatLab® (2025a) using 200 kt/y of FMR (wb) as feedstock, corresponding to approximately 550 GWh/y biomass energy input. Biomass undergoes grinding and drying before combustion in a cogeneration unit to produce heat and a CO_2-rich flue gas. Flue gas cleaning includes particulate removal, desulphurization, and dehumidification prior to cryogenic anti-sublimation CO_2 capture, assumed at 95% recovery efficiency, consistent with literature-reported performance [4].

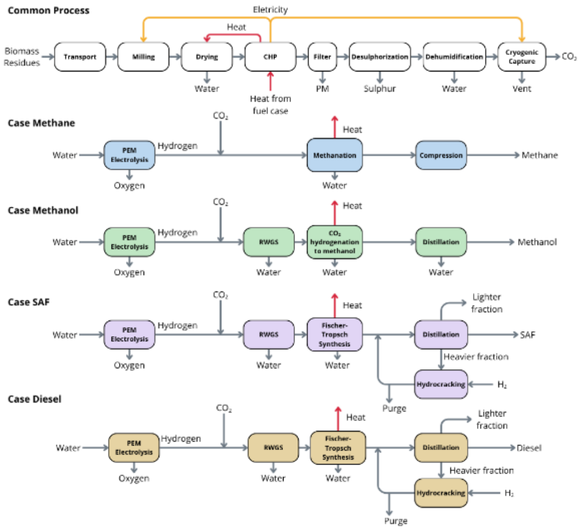

Figure 1. Considered common CO_2 capture process and respective fuel pathways.

Captured CO_2 is combined with H_2 produced via PEM electrolysis (55 kWh/kg H_2) to synthesize different fuels.

Methane is produced through Sabatier methanation, methanol via RWGS-assisted synthesis, and SAF/diesel through RWGS and Fischer–Tropsch synthesis followed by hydrocracking and distillation [5].

Economic performance was assessed through Unit Production Cost (UPC) and Levelized Cost of Fuel (LCOF) using literature-based equipment scaling correlations corrected by the Chemical Engineering Plant Cost Index (CEPCI) [6]. Sensitivity analysis (±20%) and scale analysis (50–500 kt/y wb biomass throughput) were performed to evaluate key cost drivers.

3. Results and discussion

Table 1 summarizes the main techno-economic indicators for the evaluated fuel pathways. H_2 production dominates system energy consumption in all pathways, accounting for more than 91% of total electricity demand, confirming electrolysis as the primary process bottleneck. Electrolyzer consumption ranges from 1389 to 1853 GWh/y, substantially exceeding the electricity recoverable through cogeneration and synthesis exotherms. Consequently, despite thermal integration, all scenarios remain strongly electricity dependent.

Table 1. Main techno-economic indicators of the evaluated e-fuel pathways.

Fuel	Efficiency (%)	UPC (€/kg)	LCOF (€/MWh)
Methane	36.7	2.10	154
Methanol	35.7	0.99	179
SAF	33.8	2.16	182
Diesel	32.3	2.15	196

Methanol presents the lowest mass-based production cost (0.99 €/kg) due to its comparatively simpler conversion route and lower capital burden. This indicates that methanol may perform economically better when used as a building block instead of fuel. On the other hand, when normalized by energy content, methane becomes economically preferable (154 €/MWh) because of its higher lower heating value. Conversely, SAF and diesel exhibit higher costs associated with RWGS, FT conversion, hydrocracking, and separation requirements.

Scale analysis indicates moderate cost reductions with increased biomass throughput, decreasing carbon capture cost from 191 to 139 €/tCO_2 between 50 and 500 kt/y, while fuel production costs decrease by up to 17% in FT-based pathways. However, because the system remains OPEX-dominated, economies of scale alone do not fundamentally alter cost competitiveness.

Sensitivity analysis confirms that electrolyzer specific energy consumption and electricity price are the dominant parameters influencing fuel cost, whereas biomass transport, oxygen selling price, and capture-side parameters exhibit comparatively smaller impacts.

4. Conclusions

A unified techno-economic framework for forest-based e-fuel production using biogenic CO_2 was developed and comparatively applied to methane, methanol, SAF, and diesel pathways. Results demonstrate that system performance is fundamentally constrained by H_2 production, with electrolysis dominating both electricity demand and operating costs. Methanol is the most competitive option on a mass basis, while methane becomes preferable when evaluated on an energy basis. FT-derived liquid fuels remain penalized by upgrading and separation requirements. Overall, improving renewable electricity costs and electrolysis efficiency appears substantially more relevant for competitiveness than incremental optimization of downstream capture or upgrading sections.

Acknowledgements

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Techno-economic and life cycle assessment of integrated SOEC and Fischer–Tropsch systems for synthetic fuel production from sewage sludge

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Abstract

Carbon capture, utilisation and storage (CCUS) integrated with waste-to-fuel pathways can improve carbon efficiency while producing transport fuels from organic residues. This study presents a modelling-based techno-economic and preliminary life-cycle assessment of sewage-sludge-to-liquid-fuel production by anaerobic digestion, biogas reforming, solid oxide electrolysis, reverse water-gas shift and Fischer-Tropsch synthesis. Two configurations are compared. The baseline AD-FT route reforms sewage-sludge-derived biogas, separates H_2/CO/CO_2/CH_4 by PSA, and converts conditioned syngas into gasoline, jet fuel and diesel. The upgraded AD-SOEC-FT route replaces conventional combustion with oxy-fuel combustion and uses SOEC-derived H_2 to convert captured CO_2 into CO through RWGS before FT synthesis. Results show that SOEC-RWGS integration increases liquid-fuel production and internal CO_2 utilisation, but raises electricity demand, capital cost and levelized fuel cost. The work supports CCUS-oriented process modelling cost screening and environmental evaluation of sustainable synthetic-fuel pathways for low-carbon mobility using integrated carbon capture, conversion and fuel-upgrading concepts.

Keywords: Fischer-Tropsch synthesis; sewage sludge; SOEC; carbon capture and utilisation; life cycle assessment.

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1. Introduction

Advanced liquid biofuels are increasingly considered for transport segments that are difficult to electrify, including aviation, marine transport and long-haul road freight. The European energy transition agenda also emphasises renewable energy, smart energy systems and circular-economy solutions [1]. Sewage sludge is an attractive feedstock because it is continuously generated in wastewater treatment plants and can be converted to biogas by anaerobic digestion, while the residual digestate can be further managed as a nutrient-rich stream.

Biogas-to-liquid production via Fischer-Tropsch (FT) synthesis has been studied as a route to gasoline, jet-fuel and diesel fractions, but its performance strongly depends on syngas conditioning, CO_2 management and energy integration [2-4]. Previous studies on CO_2-derived FT fuels have shown that carbon utilisation may reduce environmental impacts, although high electricity demand, capital cost and process yield remain major barriers [5,6]. Therefore, this work compares a baseline sewage-sludge-to-FT pathway with an upgraded SOEC-RWGS-assisted configuration designed for integrated CO_2 capture and utilisation.

2. Methods

The study is based on process modelling, techno-economic analysis (TEA) and preliminary life-cycle assessment (LCA). The modelling framework follows the submitted conference abstract and the detailed process model developed for the sewage-sludge-to-liquid-fuel study.

- Process simulation was carried out in Aspen Plus for the full chain from sewage sludge processing to FT fuel upgrading. The anaerobic digestion unit was parameterised using full-scale wastewater-treatment data: 248,000 t/y of sewage sludge, 604.56 kg/h of biogas, and a biogas composition of 62.26% CH_4, 36.09% CO_2 and 1.65% H_2O [7].
- In the AD-FT case, biogas is cleaned, reformed, separated in PSA units, adjusted to the required H_2/CO ratio, and converted in a low-temperature FT reactor followed by hydrocracking and distillation. Tail gases provide process heat in a conventional combustor [3,4].
- In the AD-SOEC-FT case, the conventional combustor is replaced by oxy-fuel combustion. The SOEC supplies O_2 for combustion and H_2 for RWGS, where captured CO_2 is converted to CO and recycled into the FT synthesis route [5,6].

- The TEA includes purchased-equipment scaling, CEPCI cost updating to 2025, direct and indirect cost factors, total capital investment (TCI), annual operating cost and the levelized cost of liquid fuels (LCOLF).
- The preliminary LCA uses simulation-based mass and energy balances to quantify GWP100 and compare the two configurations with a fossil liquid-fuel reference. Final LCA refinements will include sensitivity to electricity carbon intensity and allocation assumptions.

3. Results and discussion

The modelling results show that integrating SOEC and RWGS changes the role of CO_2 from a separated by-product to a carbon source for additional CO production. This increases the availability of FT-reactive carbon and improves the production of the main liquid-fuel cuts. In the upgraded configuration, gasoline, jet fuel and diesel increase by approximately 24% relative to the baseline AD-FT case, while biomethane production also increases.

Table 1. Main performance indicators of the investigated configurations.

Indicator	AD-FT	AD-SOEC-FT	Main implication
Gasoline production (kg/h)	37.52	46.63	Higher C_5-C_9 fraction
Jet-fuel production (kg/h)	57.09	70.59	Higher C_{10}-C_{13} fraction
Diesel production (kg/h)	97.68	120.90	Higher C_{14}-C_{20} fraction
Dominant electricity consumer	PSA: 182.9	SOEC: 691.6 kW	Electrical penalty
LCOLF (€/t liquid fuel)	600.55	843.58	Higher capital and operating cost
GWP100 (kg CO_2-eq.)	-0.306	0.430	Below fossil reference (0.965)

The upgraded pathway therefore provides a clear carbon-utilisation benefit, but this benefit is not obtained without penalties. Electricity consumption increases substantially, mainly because of the SOEC. The SOEC is also the largest additional capital item, reaching about 4.07 M€ in the current design. Consequently, the AD-SOEC-FT configuration improves fuel yield and CO_2 utilisation but increases the levelized cost of liquid fuels. This trade-off indicates that the upgraded pathway becomes more attractive under low-carbon and low-cost electricity, stronger carbon pricing, or when increased synthetic-fuel output is prioritised over minimum production cost.

The preliminary LCA results indicate that both sewage-sludge-based routes can perform better than the fossil liquid-fuel reference in terms of global warming impact. However, the LCA ranking is sensitive to the electricity supply assumed for SOEC operation. For this reason, the final assessment should explicitly evaluate renewable, grid-average and low-carbon electricity scenarios.

4. Conclusions

- AD-SOEC-FT increases energy efficiency from 69.52% to 71.85% but raises LCOLF from 600.55 to 843.58 €/ton.
- AD-SOEC-FT shows better environmental performance due to CO_2 utilisation via RWGS, but with higher cost.
- The main cost increase comes from SOEC and RWGSR, adding 4.07 M€ and 0.60 M€ to TCI.
- Electricity demand rises strongly from 315.7 to 1093.2 kW, mainly due to SOEC consumption.

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First Principles Life Cycle Assessment of Sustainable Aviation Fuel via Methanol to Jet with Experimental Methanol to Olefins Data Integration

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Abstract

The Methanol-to-Jet (MTJ) pathway is a promising and potentially scalable route for the production of sustainable aviation fuels (SAF), as methanol can be produced from captured CO_2 and renewable hydrogen, fitting within Carbon Capture and Utilisation (CCU) strategies. In this study, the production of jet fuel via the MTJ pathway is modelled using the Trinity College Dublin (TCD) physics constrained first principles life cycle assessment (LCA) methodology, to improve representativeness through the integration of experimental data and linking absence of data by physically authentic equations of state. The MTJ pathway consists of several processes, with this work focusing on the conversion of methanol into light olefins through the Methanol-to-Olefins (MTO) process with actual experimental data at the laboratory scale. MTO performance data obtained using a ZSM-5 zeolite catalyst synthesized in previous experimental work is integrated, replacing literature-based assumptions that carry uncertainty. In addition, a previously performed LCA of the catalyst is included within the system boundaries. Including catalyst life cycle effects increased the carbon intensity from 54.52 to 58.73 gCO_2e/MJ SAF, with catalyst manufacture and lifetime productivity emerging as the major catalytic contributors to MTJ SAF environmental performance.

Keywords: Sustainable Aviation Fuels; Methanol to Jet; Life Cycle Assessment; Zeolite; ZSM-5.

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1. Introduction

In 2023, aviation accounted for around 2.5% of global CO_2 emissions, which has generated an increasing interest in sustainable aviation fuels (SAFs) as part of the transition toward net-zero emissions by 2050. Among the different SAF pathways, Methanol-to-Jet (MTJ) has emerged as a promising alternative because it is largely based on existing technologies and can integrate renewable hydrogen and captured CO_2 within a carbon capture and utilization (CCU) framework [1].

Evaluating the environmental performance of MTJ through life cycle assessment (LCA) is essential to determine its real potential for reducing greenhouse gas emissions (GHG) compared to fossil-derived jet fuels. In particular, catalyst-related impacts are often overlooked, even though zeolites are involved in several key MTJ reaction steps. In this work, an LCA of the overall SAF production process is performed using the TCD physics-constrained first-principles LCA methodology previously reported by Mannion et al [2]. The study incorporates experimental results from the Methanol-to-Olefins (MTO) unit together with a previous LCA of the zeolite catalyst employed in this unit, which was synthesized from natural mordenite from Spain [3]. In addition, the use of real experimental conversion and selectivity data from the MTO unit allows experimentally derived process variables to be introduced into the assessment, leading to a more representative and rigorous evaluation of the overall sustainability of the MTJ pathway.

2. Methods

A physics-constrained first-principles LCA methodology previously developed by TCD [2,4] was adapted to the MTJ pathway using mass and energy balances across all process units. The system assumes the use of on-site renewable electricity, natural gas combustion for heat generation, and grey hydrogen produced via steam methane reforming.

Experimental conversion and selectivity data from the MTO unit, together with a target MTJ synthetic paraffinic kerosene (MTJ-SPK) fuel composition, were incorporated to improve process accuracy under SAF-oriented operating conditions. The environmental impact of the zeolite catalyst employed in the MTO unit was also included, considering catalyst manufacturing, regeneration behaviour, and lifetime productivity. Energy allocation was applied to distribute environmental burdens among the different products. Figure 1 shows the system boundary considered in this study, with the unit processes affected by the integration of experimental MTO data highlighted in yellow.

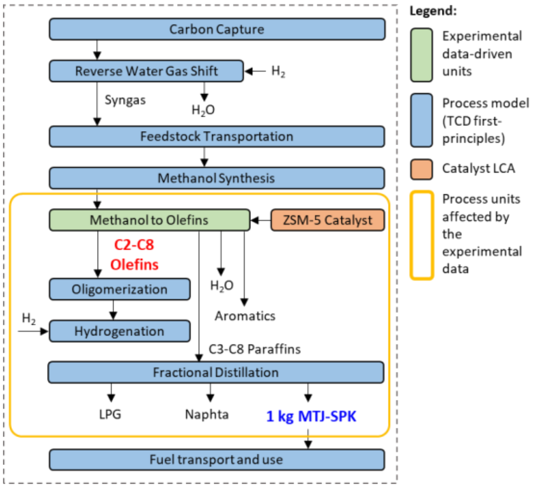

Figure 1. System diagram of the MTJ pathway for this study.

3. Results and Discussion

The incorporation of experimental MTO data into the TCD framework enabled the adaptation of the MTJ pathway towards a target SAF composition under experimentally derived process conditions. Figure 2 shows the carbon distribution of the olefin distribution produced in the MTO unit and the target paraffinic distribution required for the MTJ-SPK fuel blend.

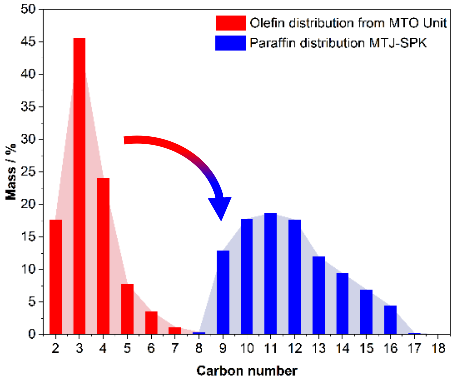

Figure 2. Carbon number distribution of the MTO unit olefin products (red) and the final MTJ-SPK paraffinic mixture (blue). The arrow symbolizes the transformation of the carbon distribution from olefins to the MTJ-SPK fuel blend (see yellow box in Figure 1).

Based on this carbon number distribution, the oligomerisation section was adjusted to favour the formation of hydrocarbons within the jet-fuel carbon range, thereby increasing SAF production relative to lighter co-products such as LPG and naphtha. As a result, a larger share of the system emissions was allocated to the SAF product stream under the energy-based allocation approach. The resulting MTJ pathway achieved life-cycle emissions of 54.5 gCO_2e/MJ_{SAF} before catalyst integration.

A key contribution of this work is the explicit incorporation of catalyst behaviour into the LCA framework through experimental reaction–regeneration data, accounting for catalyst manufacturing, regeneration, and lifetime productivity. Catalyst manufacturing (4.15 gCO_2e/MJ_{SAF}) represented the dominant contribution, while regeneration impacts (0.06 gCO_2e/MJ_{SAF}) were almost negligible. The inclusion of catalyst lifecycle effects increased the carbon intensity from 54.52 to 58.73 gCO_2e/MJ_{SAF}, corresponding to an increase of approximately 7.8%, highlighting catalyst production and durability as relevant parameters in the environmental performance of MTJ-SPK production.

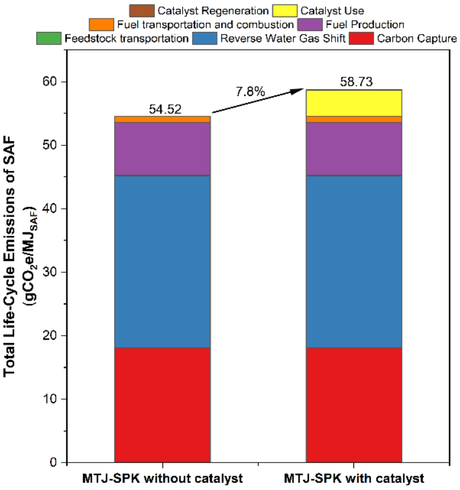

Figure 3. Total life-cycle CO_2e emissions of the MTJ process with and without MTO catalyst impacts.

4. Conclusions

The integration of experimental MTO data enhances the MTJ framework, enabling a more realistic assessment of SAF-oriented process performance. The obtained MTJ-SPK carbon intensity of 58.73 gCO_2e/MJ represents a 38% reduction compared with conventional aviation fuel (94 gCO_2e/MJ), however, it fails to comply with the 70% reduction from the ReFuelEU Aviation mandate. The inclusion of the MTO catalyst accounts for 7.8% of the total emissions, which highlights that the catalyst manufacturing and lifetime productivity can influence the carbon intensity of MTJ-SPK production and should be considered in future assessments.

Acknowledgements

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Can CO₂ Selective Membranes Improve the Techno Economic Performance of Fischer–Tropsch Synthesis?

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Abstract

Fischer–Tropsch synthesis (FTS) requires stringent control of syngas composition; however, CO_2-rich feeds can reduce reactor performance and overall process efficiency. This study investigates the techno-economic performance of integrating CO_2-selective membranes into FTS systems processing CO_2-rich syngas. Four process configurations were evaluated using Aspen Plus simulations coupled with a detailed economic assessment. Membrane integration increases carbon efficiency (up to 87%) while having a limited impact on energy efficiency. High-permeability membranes (>1000 Barrer) enable capital costs comparable to conventional recycle configurations, with similar net production costs. In contrast, upstream membrane integration shows poorer economic performance. These findings highlight the potential of membrane-based strategies to enhance carbon utilization in FTS systems.

Keywords: Fischer-Tropsch Synthesis; *CO2/CO separation*; *Techno-economic analysis*; *Process simulation*; *Sustainable fuels*

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1. Introduction

Fischer–Tropsch synthesis (FTS) requires tightly controlled syngas composition; however, CO_2 present in biogenic feeds, such as those derived from biomass gasification or CO_2 co-electrolysis, can adversely affect reactor performance, recycle requirements, and overall process efficiency [1]. Despite extensive techno-economic studies of FTS, the integration of CO_2-selective membranes —capable of selectively removing CO_2 into the permeate [2]— has not yet been assessed. Consequently, the conditions under which membrane-based approaches can compete with conventional syngas conditioning strategies remain unclear. This study aims to evaluate the technical and economic impact of membranes with varying permeabilities on FTS process performance.

2. Methods

Four configurations were evaluated (Figure 1): (i) reference FTS without recycle (REF); (ii) FTS with tail-gas recycle without syngas conditioning (REC); (iii) FTS with CO_2-selective membrane separation in the recycle loop (MEM-R); and (iv) FTS with upstream CO_2-selective membrane pretreatment of the syngas feed (MEM-P).

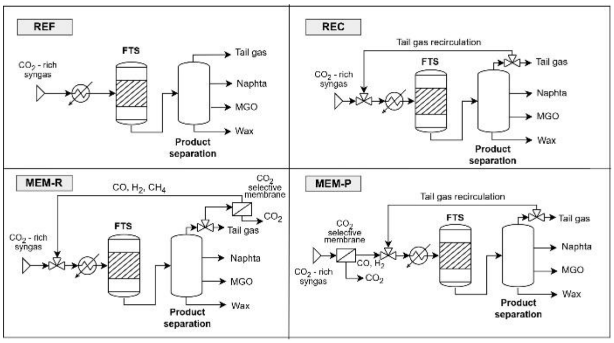

Figure 1. Process configurations studied

Simulations were performed using Aspen Plus v14. A base calc consisting of 1000 $kmol\cdot h^{-1}$ of syngas feed containing 25 mol% CO_2 was considered. Carbon (C_{eff}) and energy efficiencies (FTL_{eff}) were calculated from the mass and energy balances. The influence of CO_2-selective membrane permeability was evaluated by considering CO_2 permeabilities of 10, 100, 1000, and 5000 Barrer in cases MEM-R and MEM-P.

The techno-economic assessment was carried out following the methodology proposed by Tremel [3]. Economic indicators, including capital expenditure

(CAPEX), operating expenditure (OPEX), and net production cost (NPC), were calculated.

3. Results and discussion

Figure 2 compares C_{eff} and FTL_{eff}. The REF case exhibits the lowest carbon and energy efficiencies. The integration of membranes enhances carbon efficiency, as the separated CO_2 is considered recoverable. Among the membrane configurations, systems using lower permeability membranes (10 Barrer) achieve higher carbon efficiency due to their greater CO_2/CO selectivity, which limits CO losses. In contrast, FTL efficiency increases with CO_2 permeability, due to the the increase of CO2/H2 selectivity, which cause less loss of H2 and less requirement of H2 make up.

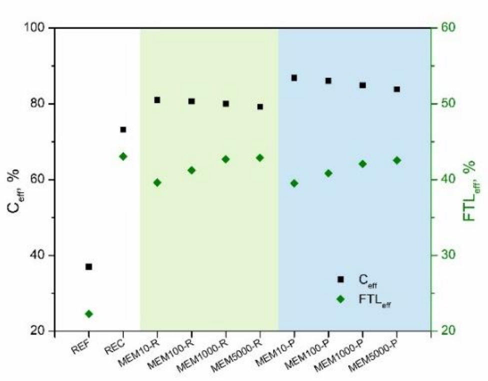

Figure 2. Carbon and Fischer-Tropsch liquid efficiency

Figure 3 compares the CAPEX of the configurations studied. Cases with 10 Barrer membranes are not presented in the graph due to excessively high costs (360 M€), driven by large membrane area requirements at low permeability. The REF case shows the lowest CAPEX. Configurations with permeability above 1000 Barrer exhibit CAPEX values comparable to the recycle case (REC).

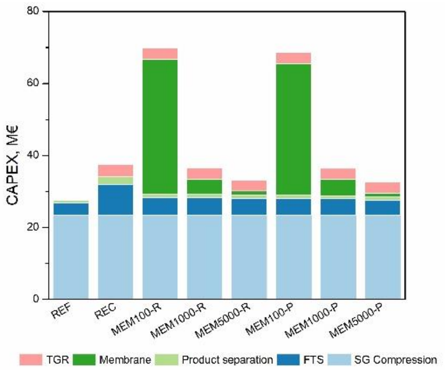

Figure 3. Capex of the different configurations in millions of euros (M€)

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Figure 4 compares the NPC of liquid fuel across configurations. Values range from 2.6 to 8 €/kg. The most competitive options are REC and high-permeability membrane systems (>1000 Barrer). Recycle configurations (MEM-R) show costs comparable to REC, whereas membrane pretreatment options (MEM-P) are slightly more expensive.

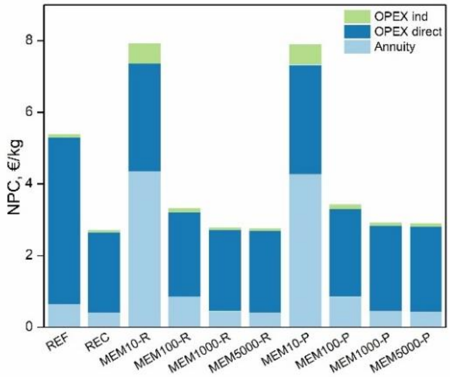

Figure 4. NPC of the different configurations

4. Conclusions

CO_2-selective membranes can improve carbon efficiency by enabling CO_2 separation and reuse, while only marginally affecting energy efficiency when high-permeability membranes (>1000 Barrer) are used, due to reduced H_2 losses. Likewise, CAPEX can be reduced because of the smaller FTS equipment required. Additionally, since the NPC is strongly influenced by process productivity, improvements in process design—particularly in the selection of separation technology—can further enhance the economic performance of the process.

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