TITLE

CAPTURING AND REUSING CO_2 AND H_2O WITH RENEWABLE ENERGY TO PRODUCE SUSTAINABLE HYDROCARBON FUELS

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INTRODUCTION

A promising strategy that addresses both environmental and energy issues is the recycling of CO_2 and H_2O with renewable energy to create sustainable hydrocarbon fuels. Carbon dioxide (CO_2) and water (H_2O) can be captured and converted into sustainable hydrocarbon fuels through innovative processes by employing renewable energy sources, such as solar or wind power. One such method is the Fischer-Tropsch synthesis, which uses a catalyst and renewable energy sources to transform CO_2 and H_2O into hydrocarbons. This approach has the potential to reduce reliance on fossil fuels and cut greenhouse gas emissions.

Prior research has concentrated on the creation of effective and affordable CO_2 and H_2O capture methods as well as the improvement of the Fischer-Tropsch process. To improve conversion efficiency and selectivity towards desired hydrocarbon products, various catalysts have been investigated. Slurry-based reactors have also drawn attention because of their capacity to process a variety of feedstocks and provide efficient mass and heat transfer during the reaction.

The Fischer-Tropsch method requires a number of steps, including the capture, purification, and conversion of CO_2 and H_2O in the presence of a catalyst. High temperatures and pressures are used in the reaction between the captured CO and H_2 (Syngas), which enables the catalyst to speed up the formation of hydrocarbon chains. As a result, fuels made of hydrocarbons may have characteristics resembling those of conventional fossil fuels, making them suitable for a variety of uses, including transportation.

The Fischer-Tropsch process benefits from using slurry-based reactors because they provide better heat management, better catalyst dispersion, and faster reaction rates. In these reactors, the liquid or gaseous reactants are mixed with a suspension of solid catalyst particles to ensure effective contact and improved overall performance.

OBJECTIVES

To improve the Fischer-Tropsch method while fostering sustainability.

To create a prototype with parameters that have been optimised for better selectivity and conversion rates.

To utilise the technology of the Solid Oxide Electrolysis Cell (SOEC) to convert CO_2 into CO and O_2.

To take advantage of waste CO as a valuable resource to maximise resource efficiency.

To through the use of novel compositions and structures, improve catalyst performance.

To create a sustainable and low-carbon energy supply, incorporate renewable energy sources (solar, wind).

To create a mass- and heat-transfer-efficient reactor system based on slurries.

To analyse the life cycle and the environmental impact to reduce the ecological footprint.

To establish a technology that is both scalable and profitable.

To create sustainable hydrocarbon fuels with CO_2, H_2O, and renewable energy.

METHODOLOGY

In this project, CO_2 is captured from flue gases or air and undergoes electrolysis using Solid Oxide Electrolysis Cell (SOEC) to produce CO and O_2. CO serves as the composing gas for syngas, while hydrogen is obtained through water electrolysis. The syngas is purified and introduced into the Fischer-Tropsch reactor, operating at 150-371°C and 0.7-41 bars. A slurry-based reactor with a cobalt-based catalyst suspending in a liquid is used, and the hydrogen to CO_2 molar ratio ranges from 0.7 to 2.5. The reaction forms long hydrocarbon chains that are separated and filtered to obtain desired products. Hydrocracking can be employed for further conversion.

Our work focuses on simulating the Fischer-Tropsch process and studying the impact of different catalyst behaviors in different reactors. We try to construct and investigate optimal flowsheet structures for the integrated Gas-to-Liquids (GTL) process, aiming for maximum syngas conversion. Iron-based and cobalt-based catalysts are considered, and the feasibility of using cost-effective iron-based catalysts in the GTL process is explored.The GTL process is analyzed using ASPEN Plus software, with detailed examination of the autothermal reforming process (ATR) using the Gibbs reactor model and Fischer-Tropsch synthesis (FTS) based on kinetic models for industrial iron and cobalt catalysts. Optimal flowsheet structures are identified based on thermal and carbon efficiency, as well as product distributions. ASPEN Plus provides a powerful tool for analyzing the GTL process, capturing real-world dynamics by considering industrial catalyst behavior. The study considers thermal efficiency and carbon efficiency, crucial indicators of energy utilization and carbon footprint. The findings assist in

the development of efficient and sustainable GTL technology, advancing process dynamics understanding.

RESULTS AND CONCLUSIONS

Optimal flowsheet structures were chosen for each catalyst based on thermal and carbon efficiency and product distributions. The cobalt-based catalyst's optimal structure involved full conversion without CO_2 removal from the FT tail gas, while the iron-based catalyst's optimal structure was a once-through concept with two series reactors and CO_2 removal from raw syngas.

The cobalt-based catalyst demonstrated a thermal efficiency to crude products of approximately 60%, while the iron-based catalyst exhibited a thermal efficiency ranging from 49% to 55%. During the FTS process, the iron-based catalyst produced CO_2, resulting in lower carbon efficiency (61% to 68%) compared to the cobalt-based catalyst (73% to 75%).

The cobalt-based catalyst exhibited higher activity and selectivity, with a greater preference for C5+ hydrocarbons (75% to 79%). In contrast, the iron-based catalyst showed a C5+ selectivity ranging from 63% to 75%.

The selection of optimal flowsheet structures for each catalyst was based on these performance parameters, as discussed in the preceding section. The table below provides a summary of the overall performance of the optimal flowsheet structures for both catalysts.

Summary of overall performance of the optimal structure for both catalysts

	GTL-Co PFR (%)	GTL-Co CSTR (%)	GTL-Fe PFR (%)	GTL-Fe CSTR (%)
Process Parameter				
Eff.% in ATR	85.87	86.84	86.78	87.07
C-eff.% to FT Liquids	72.10	74.64	67.94	61.48
C-loss in Purge Gas	6.67	5.98	1.65	3.40
Selectivity to Water	55.25	55.55	4.98	4.68
Selectivity to CO_2	–	–	45.46	45.65
Product Distribution				
CH_4	6.89	2.41	3.25	6.41
C_2–C_4 Gases	10.69	11.66	11.38	17.27
Oil	43.93	46.49	37.05	42.26
Wax	31.16	32.09	38.64	21.63
Loss	2.29	2.74	9.28	11.75
Energy Distribution				
FT Liquids	58.28	59.96	54.40	49.41
Fuel Gas	8.48	8.48	4.38	7.10
Electricity from Turbine	2.30	2.30	2.60	2.76
Heat from FT Reactor	17.99	16.98	20.86	22.33
Heat from Tail Gas	0.75	0.77	2.27	2.32
Internal Use for Heat Exchange	12.21	11.52	15.48	16.08

INNOVATION OF THE PROJECT

The project focuses on two key innovations: improving the recycling of tail gas and enhancing the efficiency of the Fischer-Tropsch process. A major aspect of our approach involves maximizing the utilization of resources by repurposing the Solid Oxide Electrolysis Cell (SOEC). Instead of solely generating oxygen from CO_2, we aim to utilize the CO byproduct as a valuable material for syngas production. This innovative strategy enhances the overall efficiency and sustainability of the process. By optimizing the recycling of tail gas and utilizing CO as a useful resource, we aim to achieve significant advancements in the Fischer-Tropsch process, contributing to a more efficient and environmentally friendly production of hydrocarbon fuels.

SCOPE FOR FUTURE WORKs

To date, our work has focused solely on software simulation. We have conducted extensive simulations to study and optimize the Fischer-Tropsch process, but we have not finalized the specific catalyst or reactor configurations. Our next step is to perform experimental work based on the results obtained from the simulations. These experiments will enable us to validate and refine our findings. Once the experimental phase is completed, we will be able to proceed with prototyping, implementing the optimized parameters and configurations determined from both the software simulations and experimental data. This iterative approach ensures that our project progresses effectively, combining simulation-based insights with real-world experimentation to develop a robust and efficient system for producing sustainable hydrocarbon fuels.