



Full Length Article

Techno-economic assessment of modified Fischer-Tropsch synthesis process for direct CO₂ conversion into jet fuel

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ARTICLE INFO

Keywords:

CO₂ utilisation
Modified Fischer-Tropsch synthesis
Jet fuel
Ex-situ water removal
Modelling & simulation
Techno-economic assessment

ABSTRACT

Direct use of CO₂ through modified Fischer-Tropsch synthesis (FTS) process presents a viable approach for the production of carbon-neutral jet fuel. However, achieving high performance for the CO₂-FTS process remains a significant challenge. Current technology can only achieve low CO₂ conversion and low jet fuel yield using tailored catalysts, which hinders the commercial deployment of direct CO₂-FTS process. This paper presents a techno-economic assessment (TEA) of jet fuel production via CO₂-FTS process at commercial-scale. Two ex-situ water removal configurations: (a) multi-stage CO₂-FTS process and (b) CO₂-FTS with tail gas recycle process were conducted to assess their potential for performance improvement. Process performance was evaluated using a model developed in Aspen Plus® linking with Aspen Custom Modeller® (ACM), while economic evaluation was carried out in Aspen Process Economic Analyzer®. The CO₂-FTS model was based on first principles and modified Anderson-Schulz-Flory (ASF) distribution. Results indicated that both ex-situ water removal configurations can significantly improve the process performance. CO₂-FTS process with 90% tail gas recycle has the best performance for both technical and economic analysis. The process achieved 85.8% CO₂ conversion and 35.6% jet fuel yield with the lowest energy demand of 4.57 MWh per tonne of produced jet fuel. Moreover, it boasts the lowest minimum selling price (MSP) of jet fuel at US\$2.6/kg despite incurring the second-highest capital expenditure cost of M\$ 451.3. A comparison of the two ex-situ water removal configurations at 61.9% and 76.5% CO₂ conversion, suggests that both processes exhibit comparable technical performances, yet the recycling of tail gas holds the potential to reduce economic costs. Consequently, this study will inspire researchers on process improvement and cost reduction of the commercial-scale CO₂-FTS jet fuel production.

1. Introduction

1.1. Background

The increasing amount of greenhouse gas (GHG) emissions has led to a global mean temperature rise of more than 1.2 °C since the pre-industrial era [1]. The International Energy Agency (IEA) has established the target of achieving net-zero CO₂ emissions by roughly mid-century so as to monitor and address the current situation [2]. Among the most difficult emissions to avoid will be those from aviation sector where energy-dense liquid fuels are required and commercially competitive substitutes are lacking [3]. According to the IEA, aviation accounted for 1.03 GtCO₂ (3.1 % total global CO₂ emissions from fossil fuel combustion) in 2019 and this value is projected to reach 1.9 GtCO₂

in 2050 [4]. Moreover, the jet fuel demand ran at 8 million barrels per day (Mbpd) in 2019 and could rise to 18 Mbpd by 2050 [5]. Therefore, developing technologies to produce sustainable aviation fuels (SAFs) (such as biofuels and synthetic fuels) is needed for decarbonising aviation [6].

CO₂ conversion can be regarded as a promising approach to produce carbon-neutral products and create a circular economy [7]. A broad range of CO₂-derived products, including synthetic fuels (e.g. gasoline and jet fuel) [8–10], chemical materials (e.g. plastics and fibers) [11,12], and building materials (e.g. cement and construction aggregates) [13,14] have been introduced in the literature. CO₂-derived fuels can serve as alternatives for hard-to-electrify transportation sectors, including heavy-duty trucks, shipping, and aviation. As these modes of transportation continue to rely partially on liquid fuels, the necessity for new pathways to produce low-carbon synthetic liquid fuels will persist

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<https://doi.org/10.1016/j.fuel.2024.133442>

Received 3 April 2024; Received in revised form 31 August 2024; Accepted 13 October 2024

Available online 25 October 2024

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Nomenclature		λ	Fitting parameter
b	Carbon number at break point	<i>Abbreviations</i>	
c	Olefin desorption rate constant	ACC	Annual capital cost
f_1 and f_2	Fractions of hydrocarbons	ACM	Aspen Custom Modeller®
k_1, k_5 and $k_{6,0}$	Kinetic constants	APEA	Aspen Process Economic Analyser
$\bar{M}$	Average molecular weight	ASF	Anderson-Schulz-Flory
M_n	Molecular weight of hydrocarbon n	CAPEX	Capital expenditures
N_{HC}	Total molar flowrate of produced hydrocarbons (kmol/hr)	FTS	Fischer-Tropsch synthesis
n_{HC_n}	Molar flowrate of hydrocarbon n (kmol/hr)	GHG	Greenhouse gas
n_i	Molar flowrate of reactant i (kmol/hr)	HC	Hydrocarbon
P_i	Partial pressure (MPa)	IEA	International Energy Agency
S_n	Selectivity of hydrocarbon n	Mbpd	Million barrels per day
W_n	Weight fraction of hydrocarbon n	MSP	Minimum selling price
X_i	Conversion of reactant i (mol%)	OPEX	Operational expenditures
x_n	Mole fraction of hydrocarbon n	RWGS	Reverse water gas shift
$Y_{Jetfuel}$	Yield of jet fuel (mol%)	SAFs	Sustainable aviation fuels
<i>Greek letters</i>		SOEC	Solid oxide electrolysis cell
α	Chain growth probabilities	TEA	Techno-economic assessment

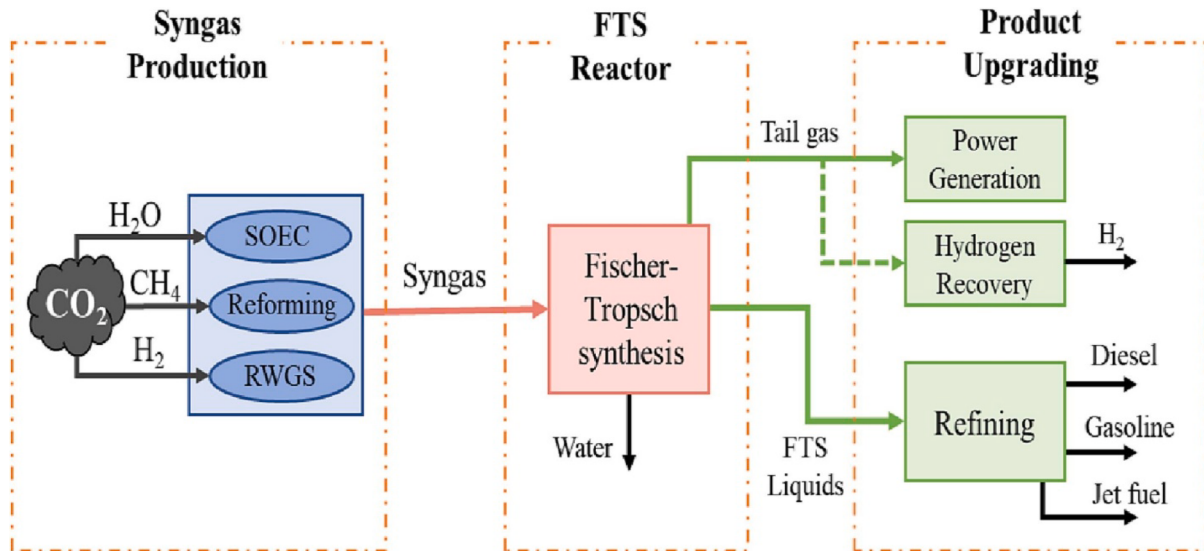


Fig. 1. Block flow diagram of a typical FTS plant [16].

Table 1

Summary of studies performed for CO₂-FTS process to jet fuel at lab-scale.

Catalyst	Operating pressure (bar)	Operating temperature (°C)	H ₂ /CO ₂ (mol/mol)	CO ₂ conversion (%)	Jet fuel (C ₈ –C ₁₆) selectivity in HC (%)	Jet fuel (C ₈ –C ₁₆) yield (%)	Ref.
CoFe-0.81Na	30	240	3	10.2	63.5	6.5	[18]
Fe-Cu	10	300	3	16.7	~37	6.2	[19]
Fe-Zn	10	340	3	34	~49	16.7	[20]
FeK/Co-NC	25	300	3	54.6	~30	16.4	[21]
Fe-Mn-K	10	300	3	38.2	47.8	18.3	[22]

[15].

CO₂ utilisation via Fischer-Tropsch synthesis (FTS) process provides the pathway to generate synthetic jet fuel. FTS process refers to as a polymerization process which uses syngas (CO and H₂) as source for the synthesis of hydrocarbon (HC) chains. Reactions (1) to (3) are possible FTS reactions to produce alkanes, olefines and alcohols products. In the indirect method (Fig. 1), there is first syngas production from CO₂

through oxide electrolysis cell (SOEC), reforming and reverse water gas shift (RWGS) followed by the FTS process in two or more reactors [16]. The one-step method, also known as the modified CO₂-FTS process has recently gained more attention as it allows the RWGS reaction (4) and FTS reactions (1) to (3) in a single reactor [17].

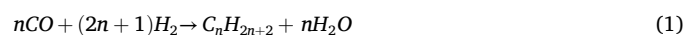
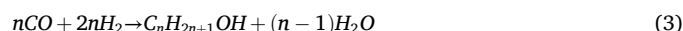


Table 2Previous studies on modelling and simulation of CO₂-FTS process to liquid fuels.

Targeted liquid fuel carbon ranges	Model	Software for model development	Assessment	Ref.
C ₅ +	Kinetic model of CO ₂ -FTS	CHEMCAD	Process analysis	[23]
FT fuel (carbon ranges NA)	Chemical equilibrium model	Aspen Plus®	TEA	[24]
Gasoline (carbon ranges NA)	Thermodynamic model	Aspen HYSYS®	Economic and environmental assessment	[25]
Gasoline (C ₅ –C ₁₁)	Steady-state CO ₂ -FTS model based on a modified ASF distribution	Aspen Plus® using Fortran® Routines	Technical analysis	[16]
Kerosene cut (C ₁₀ –C ₁₄)	Kinetic model of CO ₂ -FTS	Aspen Plus®	TEA	[26]
e-kerosene (carbon ranges NA)	Chemical equilibrium model	Aspen Plus®	Process analysis	[27]

Table 3Products and chemical reactions implemented for CO₂-FTS model.

Carbon range	Product category	Carbon number	Component	Chemical reaction
n = 1	CO Methane	1	CO CH ₄	CO ₂ + H ₂ → CO + H ₂ O CO + 3H ₂ → CH ₄ + H ₂ O
2 ≤ n ≤ 4	Light HCs (C ₂ –C ₄)	2, 3 and 4	C ₂ H ₆ C ₂ H ₄ C ₃ H ₈ C ₃ H ₆ C ₄ H ₁₀ C ₄ H ₈	2CO + 5H ₂ → C ₂ H ₆ + 2H ₂ O 2CO + 4H ₂ → C ₂ H ₄ + 2H ₂ O 3CO + 7H ₂ → C ₃ H ₈ + 3H ₂ O 3CO + 6H ₂ → C ₃ H ₆ + 3H ₂ O 4CO + 9H ₂ → C ₄ H ₁₀ + 4H ₂ O 4CO + 8H ₂ → C ₄ H ₈ + 4H ₂ O
5 ≤ n ≤ 7	C ₅ –C ₇ HCs	5, 6 and 7	C ₅ H ₁₂ C ₅ H ₁₀ C ₆ H ₁₄ C ₆ H ₁₂ C ₇ H ₁₆ C ₇ H ₁₄	5CO + 11H ₂ → C ₅ H ₁₂ + 5H ₂ O 5CO + 10H ₂ → C ₅ H ₁₀ + 5H ₂ O 6CO + 13H ₂ → C ₆ H ₁₄ + 6H ₂ O 6CO + 12H ₂ → C ₆ H ₁₂ + 6H ₂ O 7CO + 15H ₂ → C ₇ H ₁₆ + 7H ₂ O 7CO + 14H ₂ → C ₇ H ₁₄ + 7H ₂ O
8 ≤ n ≤ 16	Jet Fuel (C ₈ –C ₁₆)	12	C ₁₂ H ₂₆ C ₁₂ H ₂₄	12CO + 25H ₂ → C ₁₂ H ₂₆ + 12H ₂ O 12CO + 24H ₂ → C ₁₂ H ₂₄ + 12H ₂ O
n ≥ 17	Wax	20	C ₂₀ H ₄₂	20CO + 41H ₂ → C ₂₀ H ₄₂ + 20H ₂ O



1.2. Literature review

The products from the modified CO₂-FTS process can be wide since a variety of catalysts can be used. This paper (hence, the literature review) focuses on the synthesis of jet fuel from CO₂-FTS process. To date, the modified CO₂-FTS process for CO₂ conversion into jet fuel has only been reported at laboratory scale. A summary of a few studies on the CO₂-FTS process to jet fuel (C₈–C₁₆) is presented in Table 1. Most studies reported Fe and Co-based catalysts and achieved up to 64 % selectivity to jet fuel whereas, CO₂ conversion varies from 10 % to 55 % [18–22]. The largest jet fuel yield of 18.3 % can be found from Yao et al. [22].

Table 2 presents an overview of previous studies on modelling and simulation for the modified CO₂-FTS process to liquid fuels. Meier et al. [23] developed a kinetic model comprising 20 reactions to study CO₂-FTS plant performance through periodical removal of water for C₅ hydrocarbons. The authors looked into ex-situ water removal to improve CO₂-FTS reaction rates and C₅ + selectivity. Zang et al. [24] assessed the synthesis of liquid fuels (C₅+) through a techno-economic assessment (TEA) of the CO₂-FTS process and predicted the minimum selling price (MSP) of the FT fuel is \$5.4–5.9/gal (throughout this paper, \$ always refers to USD). Fernandez-Torres et al. [25] applied Aspen-HYSYS® to design and optimise CO₂-FTS to gasoline at commercial-scale. For a gasoline production rate of 23.65 ton/hr, their results indicated that the capital expenditures (CAPEX) and operational expenditures (OPEX) are in the ranges of 73 to 128 M\$ and 244 to 1951 M\$/yr, respectively. Kamkeng and Wang [16] studied the performance improvement of the CO₂-FTS process for gasoline (C₅–C₁₁) production using ex-situ water removal. The authors developed a CO₂-FTS model based on first principles and a modified Anderson-Schulz-Flory (ASF) distribution, which was implemented in Aspen Plus® using Fortran® Routines and validated with laboratory data. The results demonstrated that the use of ex-situ water removal technique can increase CO₂ conversion and gasoline yield by up to 34 % and 70 %, respectively. The single CO₂-FTS reactor with recycle and three-stage CO₂-FTS reactors in series showed a similar process efficiency of 66.4 %. However, economic analysis was not evaluated to indicate the feasibility of commercial deployment. Colelli et al. [26] carried out the comparative TEA for the indirect and direct production of synthetic kerosene (C₁₀–C₁₄) via FTS. They predicted the productivity of the plant (66.18 bbl/d and 38.46 bbl/d) and product cost (460 to 1435 €/bbl and 752 to 2364 €/bbl) for the indirect and direct process. However, their simulation results based on kinetic model present very large relative errors (–38.6–77.8 %) compared with experimental data. Atsonios et al. [27] investigated four different thermochemical pathways for CO₂ conversion into synthetic kerosene using chemical equilibrium models developed in Aspen Plus®. They indicated that the low-temperature CO conversion through RWGS and FTS is the most energy efficient pathway, but the economic evaluation is not included for comparison.

1.3. Aim and novel contributions of this paper

In this study, a TEA was carried out for direct CO₂ conversion into jet fuel (C₈–C₁₆) via CO₂-FTS process at commercial scale. Two ex-situ water removal configurations were considered for jet fuel yield improvement. This study provides the following novel contributions:

- (1) This study proposes an advanced model based on first principles and a modified ASF for jet fuel production from CO₂-FTS process. The CO₂-FTS model was implemented in Aspen Plus® linking

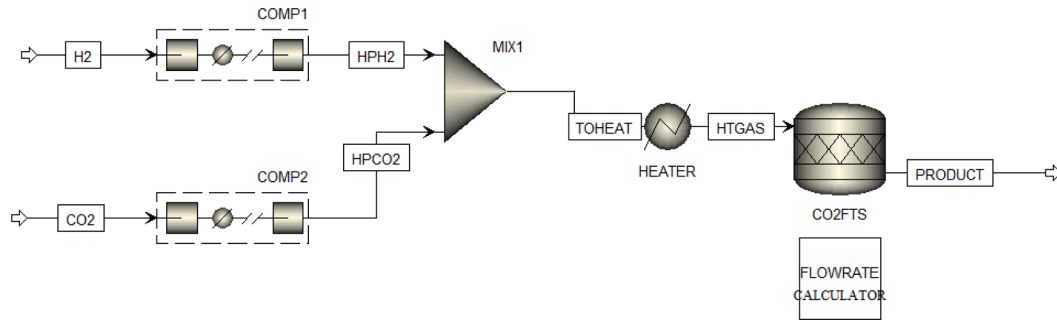


Fig. 2. Flowsheet diagram of CO₂-FTS process implemented in Aspen Plus® using Fortran® Routines.

Table 4

Input parameters used for model validation.

Parameter	Value	Reference
Reactor type	fixed bed	[22]
Reactor diameter (cm)	1	
Reactor temperature (°C)	300	
Reactor pressure (MPa)	1	
H ₂ /CO ₂ ratio	3	
Flow rate (mL/min)	40	
CO ₂ conversion (%)	38.2	
Chain growth probability	a_1	0.79
	a_2	0.57
Carbon number at breakpoint	12	
Kinetic constants	k_1	1.66×10^{-2}
	k_5	6.99×10^{-5}
	$K_{6,0}$	2.02×10^{-2}
Constant c	-0.26	
Fitting parameter λ	$n \leq 7$	$0.15e^{0.35n}$
	$8 \leq n \leq 12$	$0.29e^{0.39n}$
	$n \geq 13$	$2.7e^{36n^{-1}}$

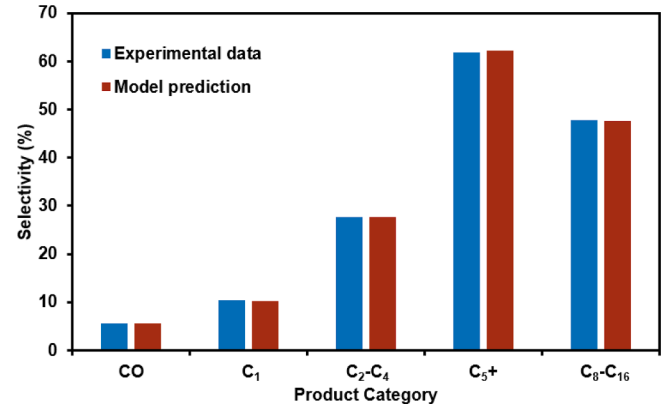


Fig. 4. Model prediction and experimental values of CO₂-FTS product selectivity.

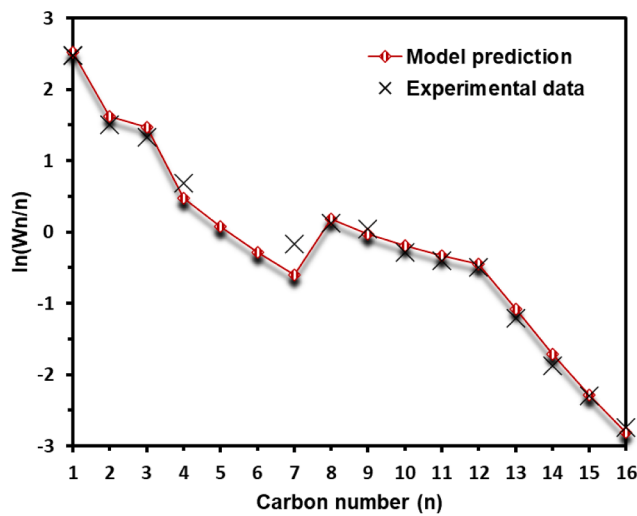


Fig. 3. Model prediction of ASF plot compared with experimental data.

with Aspen Custom Modeller® (ACM) and validated using experimental data [22].

- (2) Although ex-situ water removal has been previously considered for CO₂-FTS process improvement [16,23], this technique has never been applied for CO₂-FTS to jet fuel. Therefore, this study looks into two ex-situ water removal configurations (reactors in series and a single reactor with recycle) assess its potential in performance improvement during jet fuel production through the CO₂-FTS process.

Table 5

Model validation results of selectivity for different product category.

Product category	Selectivity (%) Experimental data	Model prediction	Relative error (%)
CO	5.6	5.60	0.00
C ₁	10.4	10.14	-2.51
C ₂ -C ₄	27.7	27.60	0.34
C ₅ +	61.9	62.26	0.58
C ₈ -C ₁₆	47.8	47.64	-0.34

- (3) A comparative TEA is carried out for the two ex-situ water removal configurations of the CO₂-FTS process. This analysis aims to provide with relevant information to decision-makers on the commercial application of jet fuel produced from CO₂-FTS process.

2. Model development and validation of CO₂-FTS process

2.1. Model development

2.1.1. Assumptions

The following assumptions were made during CO₂-FTS model development:

- CO₂-FTS process operates at steady-state condition. Hence, the accumulation of heat and mass was not considered.
- Only reactant conversion and specific products are considered based on material balance and stoichiometric reactions.
- The type of HCs depends on the nature of catalyst. Since the selectivity towards oxygenated compounds was below 1.0 % during experiments [22], they were neglected in this model. Hence, only olefins and paraffins were considered in this model.

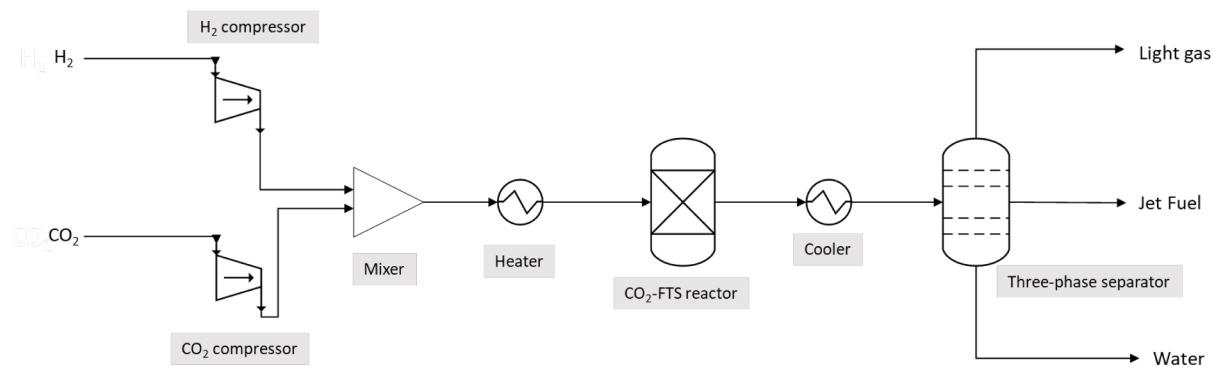


Fig. 5. Base case scenario of the CO₂-FTS plant for jet fuel production.

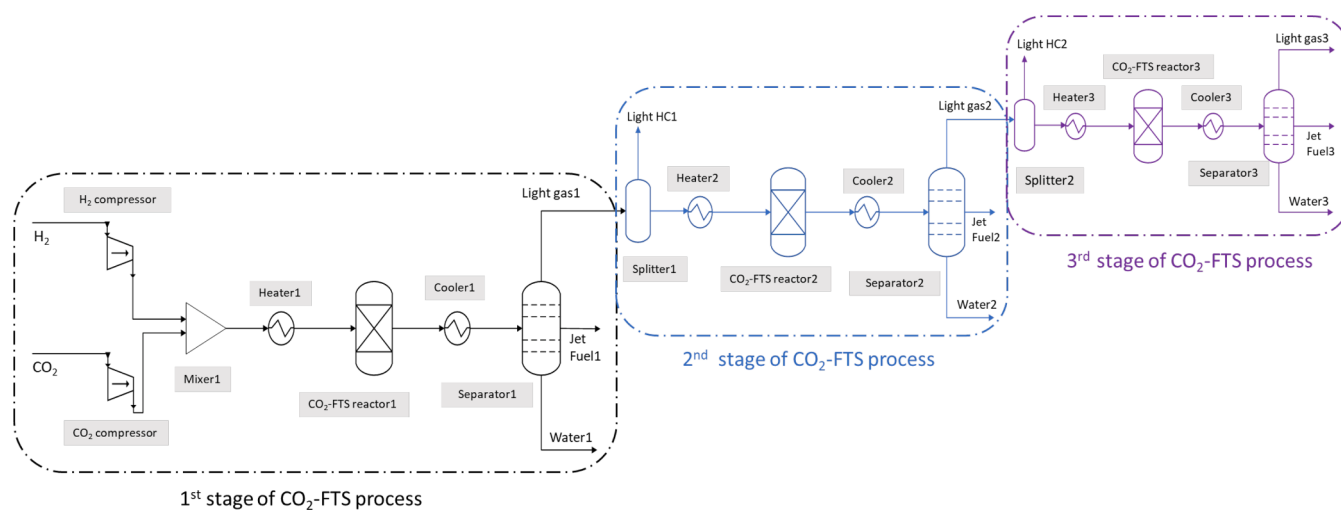


Fig. 6. Multi-stage CO₂-FTS plant for jet fuel production.

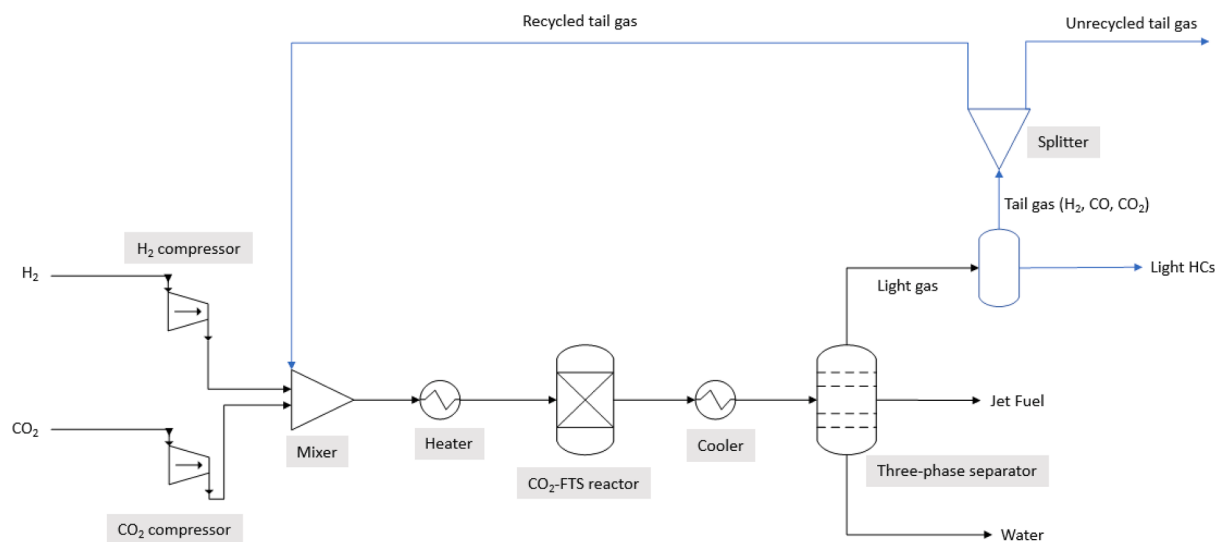


Fig. 7. CO₂-FTS with tail gas recycle plant for jet fuel production.

- The chain growth probability of hydrocarbons was based on given Anderson-Schulz-Flory (ASF) plot from experiments [22].
- The large number of CO₂-FTS reactions was handled by lumping technique. It is simply defined as grouping several components into a smaller number of components to represent the whole group [28].

2.1.2. Modelling of hydrocarbon distribution

A model for the prediction of hydrocarbon distribution was developed in ACM. This model combines modified ASF theory and kinetic modelling of CO₂-FTS process to accurately predict the hydrocarbon distributions. Based on the previous modified ASF model, the weight fraction of hydrocarbon (W_n) was calculated from Eq. (5) [29] based on

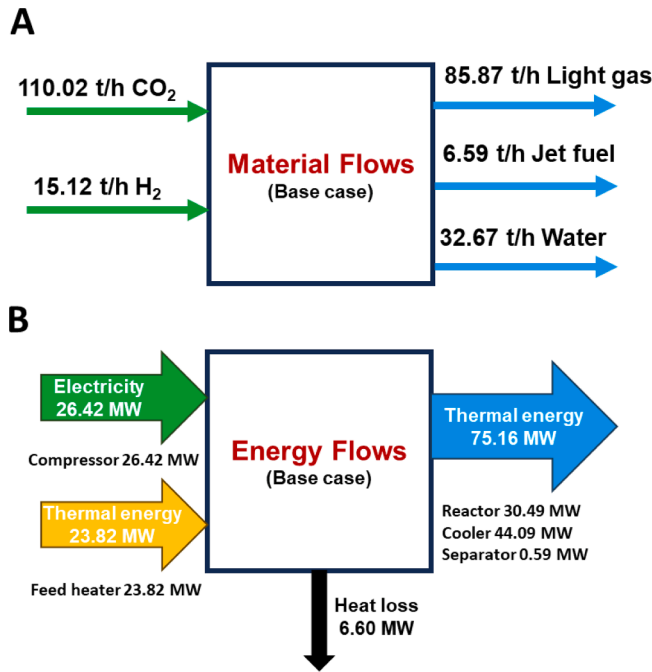


Fig. 8. Material and energy flows of base case.

Table 6
Performance summary of the base case CO₂-FTS process.

Parameter	Value
Jet fuel features	
Mass flowrate (tonne/h)	6.59
Density at 15 °C (kg/m ³)	741.89
Viscosity at -20 °C (mm ² /s)	2.70
Flash point (°C)	77.37
Energy consumption (MW)	
Compressors	26.42
Feed heater	23.82
Reactor cooling jackets	30.49
Syn crude coolers	44.09
Flash drums	0.59
Heat losses	6.60
Energy input (MW)	50.24
Total energy consumption (MW)	132.00
Energy consumption for each tonne captured CO ₂ (kWh/t-CO ₂)	456.67
Energy consumption for each tonne produced jet fuel (MW/t-Jet fuel)	7.62
CO ₂ conversion (mol%)	38.20
Jet fuel yield (mol%)	17.18

two chain growth probabilities (α_1 and α_2) and two fractions of hydrocarbons (f_1 and f_2).

$$W_n = f_1 \times \alpha_1^{n-1} + f_2 \times \alpha_2^{n-1} \quad (5)$$

The C₃ hydrocarbon is considered a deviation from the standard ASF distribution due to the complex reaction mechanisms of the Fe-Mn-K catalyst used. Consequently, specific experimental conditions and kinetic values were employed to accurately model the chain growth probability and weight fraction for C₃ hydrocarbons. The chain growth probability of C₃ (α_{C_3}), as shown in Eq. (6), was calculated using the specific experimental conditions (P_{CO_2} and P_{H_2}) and kinetic values (k_1 , k_5 and $k_{6,0}$) suggested by Kamkeng and Wang [16].

$$\alpha_{C_3} = \frac{k_1 P_{CO_2}}{k_1 P_{CO_2} + k_5 P_{H_2} + k_{6,0} e^{3c}} \quad (6)$$

The weight fraction of C₃ compounds (W_3) can be calculated from Eq. (7) using chain growth probability of C₃.

$$W_3 = 3 \times (1 - \alpha_{C_3})^2 \times \alpha_{C_3}^2 \quad (7)$$

Two fractions of hydrocarbons (f_1 and f_2) related to α_1 and α_2 are derived from Eqs. (8) and (9) based on carbon number at break point (b) and fitting parameter (λ).

$$f_1 = \lambda \frac{1 - W_3}{\frac{1}{1 - \alpha_1} - \frac{\alpha_1}{1 + \alpha_1} + \left[\frac{1}{1 - \alpha_2} - \frac{\alpha_2}{1 + \alpha_2} \right] \left(\frac{\alpha_1}{\alpha_2} \right)^{b-1}} \quad (8)$$

$$f_2 = f_1 \times \left(\frac{\alpha_1}{\alpha_2} \right)^{b-1} \quad (9)$$

The mass fraction of hydrocarbons obtained from ASF theory is converted into corresponding selectivity (S_n) by applying Eqs. (10)–(12).

$$\frac{1}{\bar{M}} = \sum_{n=1}^{50} \frac{W_n}{M_n} \quad (10)$$

$$x_n = \frac{W_n}{M_n} \times \bar{M} \quad (11)$$

$$S_n = \frac{x_n \times n}{\sum_{n=1}^{50} x_n \times n} \quad (12)$$

where M_n is the molecular weight of hydrocarbon n , $\bar{M}$ is the average molecular weight, and x_n is the mole fraction of hydrocarbon.

With the obtained selectivity of hydrocarbons, the molar flowrate for each carbon compounds (n_{HC_n}) are calculated based on Eqs. (13) and (14).

$$N_{HC} = n_{CO_{2in}} \times X_{CO_2} \times X_{CO} \quad (13)$$

$$n_{HC_n} = N_{HC} \times \frac{S_n}{n} \quad (14)$$

where N_{HC} is the total molar flowrate of produced hydrocarbons, X_i is the conversion of reactant i , and n_i is molar flowrate of reactant i .

2.1.3. Model implementation of CO₂-FTS process using Aspen Plus® linking with Aspen customer modeller®

The CO₂-FTS process was implemented in Aspen Plus® linking with ACM. Initially, the modified ASF distribution model was calculated in ACM® for every carbon number ranging from 1 to 50. The CO₂-FTS reactions and lumping components used for process modelling are presented in Table 3. For simplicity, the wax category represents hydrocarbons with carbon numbers greater than 17, encompassing both waxes and any minimal higher-carbon components such as diesel. Based on the olefin to paraffin ratio specified in the experimental study, the flowrate of the corresponding carbon number can determine each product.

Fig. 2 illustrates the CO₂-FTS process flowsheet implemented in Aspen Plus® using the physical property method Peng-Robinson. The ACM model was exported as a calculation block (FLOWRATE) to Aspen Plus® flowsheet for calculating the flowrate of hydrocarbons presented in Table 3. With the help of Fortran® Routines, the PRODUCT stream is correlated to ACM model. The feedstock H₂ and CO₂ were assumed to be at 25 °C and 1 bar. They are first compressed at 10 bar with a 2-stage compressor featuring intercooling. Afterwards, they were mixed and heated at 300 °C in a heater (HEATER). The CO₂-FTS reactor which performs the RWGS and FTS reactions is represented by a stoichiometry reactor block (CO₂-FTS) in Aspen Plus®.

2.2. Model validation

To validate the developed CO₂-FTS model, lab-scale experiments conducted at the University of Oxford were used. The experiments provide ASF plots and selectivity for different carbon categories for model validation. The ratio of olefin to paraffin for each hydrocarbon is obtained from experiments [18,22]. The input process conditions and

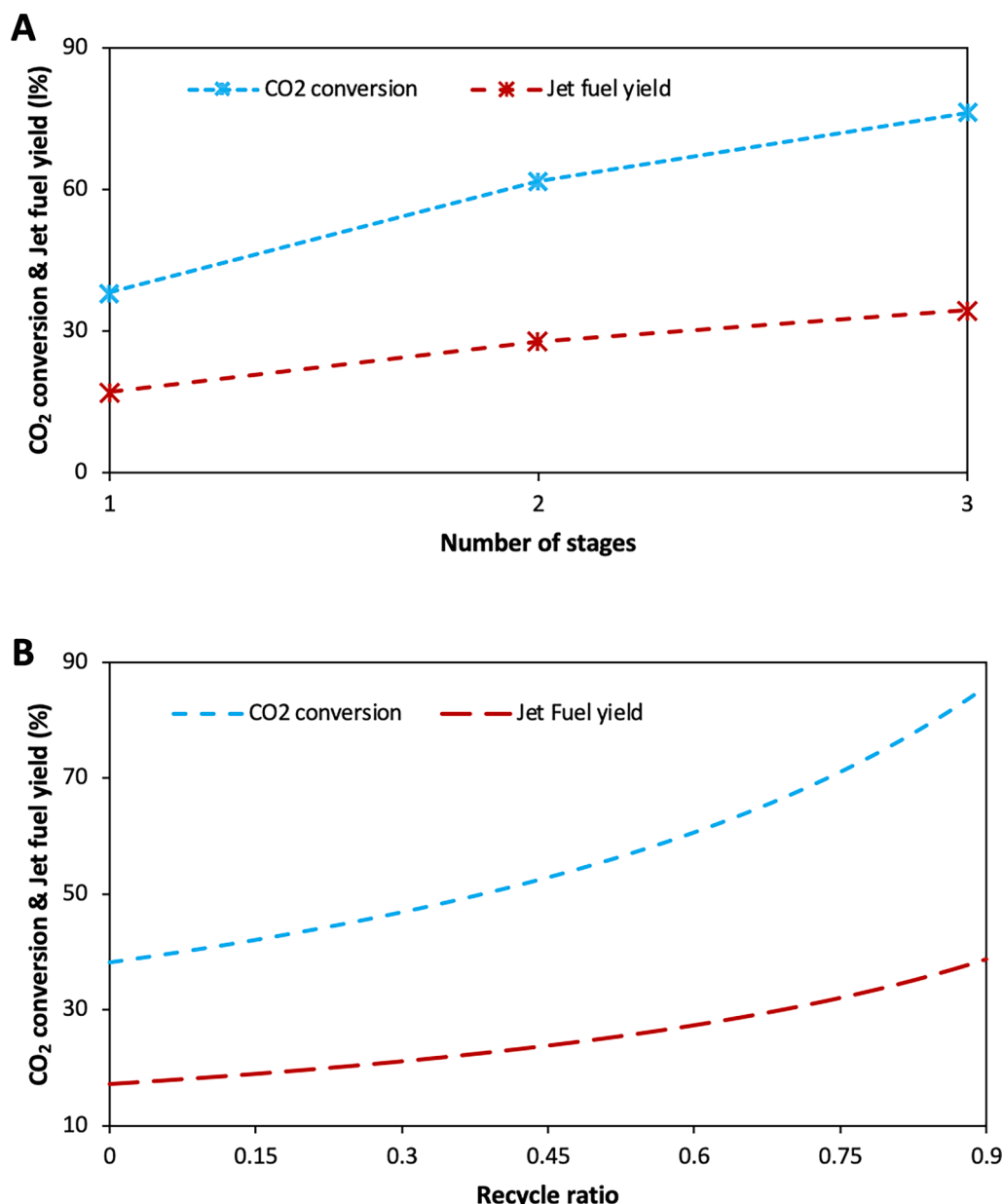


Fig. 9. Performance prediction of CO₂ conversion and jet fuel yield for CO₂-FTS process under two ex-situ water removal configurations: (A) Multi-stage CO₂-FTS process, and (B) CO₂-FTS with tail gas recycle.

parameters used for the CO₂-FTS model validation are presented in Table 4. Process conditions were available from Yao et al. [22], other parameters were reasonably assumed based on literature.

Fig. 3 compares the model prediction results of the ASF plots with the experimental data given from carbon numbers 1 to 16. The ASF plots agree with the experimental trend and model values. On the other hand, Fig. 4 compared five product categories of model prediction results with experimental data. All the relative errors shown in Table 5 are below 2.5 %. Therefore, Figs. 3 and 4 show great agreement of the developed model with experimental work.

3. Simulation of the modified CO₂-FTS process for jet fuel production at commercial scale

3.1. Base case scenario

The base case scenario is the CO₂-FTS process using a single reactor. The process features an open-loop configuration without the

recirculation or upgrade of unconverted reactants, water removal and/or reactor design. The results obtained from the base case scenario were used as a reference for performance comparison between the optimised plants.

The process flow diagram of the base case scenario developed in Aspen Plus® linking with ACM is shown in Fig. 5. The inlet flowrate of CO₂ and H₂ were chosen 110.02 t/h and 15.12 t/h, respectively. This was based on commercial CO₂ utilisation plant in previous studies [16,25]. In the base case scenario, the products leaving the reactor are cooled down to 40 °C according to industry operation for syncrude oil separation. Finally, a three-phase separator divides the stream into light gas, jet fuel and water.

3.2. Ex-situ water removal configurations for CO₂-FTS process

Previous studies (both experimental and modelling) have demonstrated that water formation during CO₂-FTS process significantly inhibits CO₂ conversion due to a decrease in the driving force of the RWGS

Table 7Performance summary of the multi-stage CO₂-FTS process.

Parameter		Two-stage	Three-stage
Jet fuel features	Mass flowrate (tonne/h)	11.07	13.86
	Density at 15 °C (kg/m ³)	741.55	741.31
	Viscosity at −20 °C (mm ² /s)	2.67	2.65
	Flash point (°C)	77.36	77.35
Energy consumption (MW)	Compressors	26.42	26.42
	Feed heater	38.41	47.05
	Reactor cooling jackets	51.59	64.75
	Syncrude coolers	71.82	88.62
	Flash drums	0.98	1.23
	Heat losses	9.96	12.00
Energy input (MW)		64.83	73.47
Total energy consumption (MW)		199.19	240.07
Energy consumption for each tonne captured CO ₂ (kWh/t-CO ₂)		589.25	667.78
Energy consumption for each tonne produced jet fuel (MW/t-Jet fuel)		5.86	5.30
CO ₂ conversion (mol %)		61.86	76.46
Jet fuel yield (mol %)		27.82	34.38

Table 8Performance summary of CO₂-FTS with tail gas recycle process.

Parameter		63.8 % recycle	80.3 % recycle	90 % recycle
Jet fuel features	Mass flowrate (tonne/h)	11.33	13.83	15.94
	Density at 15 °C (kg/m ³)	741.32	740.75	739.41
	Viscosity at −20 °C (mm ² /s)	2.65	2.60	2.48
	Flash point (°C)	77.36	76.91	69.00
Energy consumption (MW)	Compressor	26.42	26.42	26.42
	Pre-heater	23.82	38.47	44.61
	Reactor cooling jackets	52.78	64.28	73.46
	Syncrude coolers	72.62	85.94	93.67
	Flash drums	1.01	1.23	1.41
	Heat losses	10.07	11.71	12.71
Energy input (MW)		64.90	71.03	72.92
Total energy consumption (MW)		201.37	234.19	254.17
Energy consumption for each tonne captured CO ₂ (kWh/t-CO ₂)		589.85	645.63	662.78
Energy consumption for each tonne produced jet fuel (MW/t-Jet fuel)		5.73	5.14	4.57
CO ₂ conversion (mol %)		61.86	76.46	85.82
Jet fuel yield (mol %)		27.82	34.38	35.59

reaction. Therefore, continuous water removal is essential to improve RWGS reaction rate hence, CO₂ conversion.

3.2.1. Multi-stage CO₂-FTS process

Fig. 6 depicts the concept of a multi-stage CO₂-FTS process, which is created by connecting continuous stages of CO₂-FTS process in series. This multi-stage design incorporates multiple CO₂-FTS reactors by re-using unreacted feedstocks from previous stages. The process was simulated in Aspen Plus® linking with ACM. Although several stages can be interconnected, this paper only investigated two-stage and three-stage for the CO₂-FTS process.

In a typical three-stage CO₂-FTS process, the first stage corresponds the base case scenario aforementioned. The second and third stages employ the same process as the base case but exclude compressors and incorporates additional separators to split light hydrocarbons. For the first stage, the feed stream contains only H₂ and CO₂ to the CO₂-FTS reactor while for the second and third stages, the feed stream also includes unconverted CO₂, H₂ and CO. The operating conditions for each stage were same as the base case process shown in Table 4.

3.2.2. CO₂-FTS with tail gas recycle process

The ex-situ water removal for CO₂-FTS process through tail gas recycle (Fig. 7) was also simulated in Aspen Plus® linking with ACM. In

comparison to the base case process, the tail gas (unreacted H₂, CO, and CO₂) is separated from the light gas and recycled to the mixer. The recycled tail gas flowrate depends on the recycle ratio set in the splitter. The splitter separates tail gas with H₂ to CO₂ ratio of 3 to meet the strict operating condition under Fe-Mn-K catalyst. Since only the ratio of 3 is studied in the experiments, the other ratio of the reaction circumstance is unknown. The study of different recycle ratio is carried out by sensitivity analysis in Aspen Plus®. It should be noted that the recycle ratio was initially set from 0 to 100 %. However, only 0–90 % can be realised in Aspen Plus® due to the convergence of software. The recycled tail gas is mixed with the feedstock before preheating in the heater. Unrecycled tail gas and light hydrocarbons is not considered for further application.

4. Technical analysis of the modified CO₂-FTS process for jet fuel production at commercial scale

4.1. Assumptions and performance metrics

Process analysis of CO₂-FTS process was performed under the following assumptions.

- The CO₂-FTS reactor and Fe-Mn-K catalyst behave the same way at lab-scale and commercial-scale.
- 5 % heat losses were assumed during whole CO₂-FTS operating units [16].
- No pressure drop was assumed in the heaters and coolers.
- CO₂ conversion (X_{CO_2}) and jet fuel yield ($Y_{Jetfuel}$) are calculated based on Eqs. (15) and (16).

$$X_{CO_2} = \frac{nCO_{2in} - nCO_{2out}}{nCO_{2in}} \quad (15)$$

$$Y_{Jetfuel} = X_{CO_2} \times S_{Jetfuel} \quad (16)$$

4.2. Base case scenario

The results of the material and energy balance of the base case CO₂-FTS process are shown in Fig. 8. The base case CO₂-FTS plant leads to roughly 6.59 t/h of jet fuel, 85.87 t/h of light gas and 32.67 t/h of water (Fig. 8A). Fig. 8B shows the total energy input (26.42 MW electricity and 23.82 MW thermal energy) to the system, the energy output from the system (75.16 thermal energy), and the assumed heat loss (6.60 MW). Note that most of the thermal energy output is from cooling energy (30.49 MW reactor cooling jackets and 44.09 MW syncrude cooler). Compared to the previous study by Kamkeng and Wang [16], total energy in this study is reduced by 23.35 MW. This is mainly due to the lower energy consumption in the compressors (26.42 MW compared to 70.79 MW). In fact, for the jet fuel production the operating pressure is only 10 bar which is one third of the gasoline production [16].

The performance summary is presented in Table 6 which shows jet fuel characteristics, energy consumption for each sector, CO₂ conversion and jet fuel yield. The direct CO₂-FTS process achieves a jet fuel selectivity of 47.6 %, however the jet fuel yield is only 17.2 % due to low CO₂ conversion (38.2 %). Considering the selectivity towards C₁₇₊ hydrocarbons is roughly 2.0 %, for simplicity, the distillation and hydrocracking processes were not considered [16]. The energy consumption for feedstock of CO₂ and the product of jet fuel were calculated and respectively are 456.67 kWh per ton of feedstock CO₂ and 7.62 MW per ton of produced jet fuel. The density of jet fuel was found 742 kg/m³ from the model which is close to the synthetic paraffinic kerosene (749 kg/m³) from previous literature [31]. However, these values are lower than the commercial jet fuels Jet A and Jet A-1 (775–840 kg/m³) [32]. This could be due to the absence of aromatic compounds in the produced jet fuel. For future commercialisation to reach the standard jet fuel density level, further approaches can be adopted, such as adding appropriate fuel additives and blending with conventional jet fuel [33].

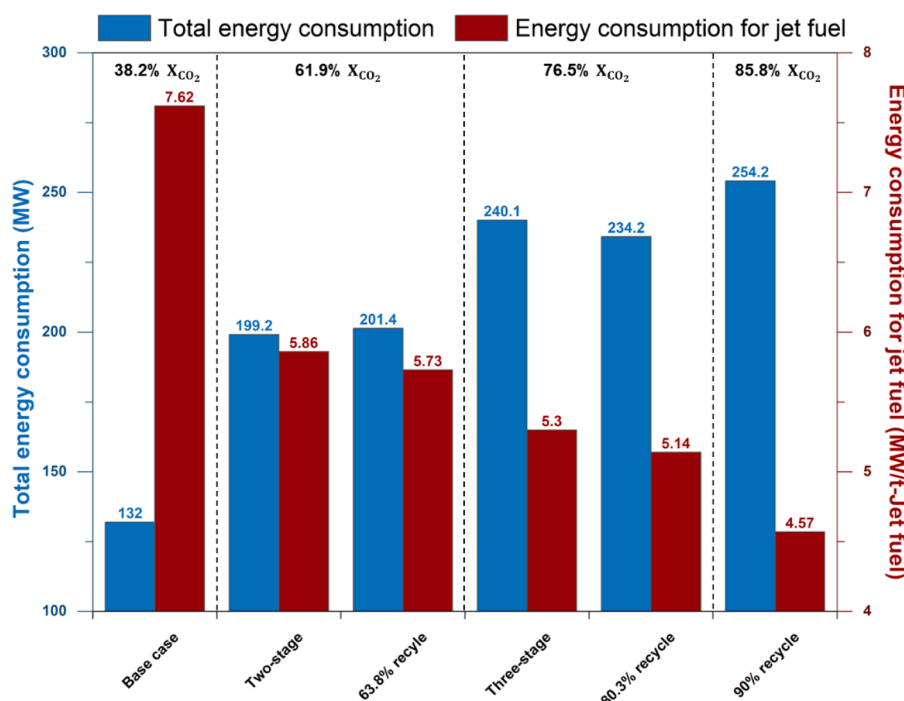


Fig. 10. Summary of energy consumption for different CO₂-FTS process.

Table 9

Financial parameters used in economic analysis.

Parameter	Value	Reference
CO ₂ price (\$/kg)	0	[35]
H ₂ price (\$/kg)	2	[36]
Heating price (\$/GJ)	4.25	[34]
Cooling water utility cost (\$/tonne)	0.35	[34]
Electricity price (\$/kWh)	0.0775	[34]
Operating time per year (hour)	8000	[34]
Plant lifetime (year)	20	[25]
Interest rate (%)	10	[25]

4.3. Performance prediction for the ex-situ water removal configurations

4.3.1. CO₂ conversion and jet fuel yield

Fig. 9 shows the predicted trends of using multi-stage CO₂-FTS process and CO₂-FTS with tail gas recycle process. Both ex-situ water removal configurations show improvement in CO₂ conversion and jet fuel yield. With the addition of the number of stages, the CO₂ conversion increases from 38.2 % to 61.9 % at two stages and 76.5 % at three stages. On the other hand, recycling 90 % tail gas achieved 85.8 % CO₂ conversion and 35.6 % jet fuel yield. With the design specification method in Aspen Plus®, two recycle ratio points (63.8 % and 80.3 %) were calculated, corresponding to the same CO₂ conversion in the two-stage and three-stage CO₂-FTS process. From the standpoint of improving CO₂ conversion and jet fuel yield, adding the number of stages to the CO₂-FTS process and adopting tail gas recycling have the same function.

4.3.2. Energy consumption

With the improvement in CO₂ conversion and jet fuel yield, the energy consumption also increased for both ex-situ water removal configurations. Tables 7 and 8 present the performance summary for the multi-stage CO₂-FTS process and CO₂-FTS with tail gas recycling. The multi-stage CO₂-FTS process showed 1.7 times increase in jet fuel productivity for the two-stage process and 2.1 times increase for the three-stage process, respectively. The energy demand for compressors remains the same because feedstock is compressed only in the first stage. The

increase in the total energy demand is mainly due to the thermal energy demand in the 2nd and 3rd stages of the CO₂-FTS process. Although the total energy consumption and the energy consumption per ton of feedstock CO₂ increase with the addition of stages to the CO₂-FTS process, the energy consumption per ton of jet fuel produced decreases. The same performance trends were found for the tail gas recycle case. As the recycle rate increases, the total energy demand rises while the energy demand for each ton of jet fuel produced decreases.

4.3.3. Comparison between two ex-situ water removal configurations

To find out the energy consumption between the two ex-situ water removal configurations, they were compared at the same CO₂ conversion (61.9 % and 76.5 %). Therefore, in Fig. 10, the two-stage CO₂-FTS process is compared to the CO₂-FTS process with 63.8 % tail gas recycle, and the three-stage CO₂-FTS process is compared to the CO₂-FTS process with 80.3 % tail gas recycle. The tail gas recycle process consumed more total energy at 61.9 % CO₂ conversion compared to the multi-stage process, while the result is reversed at 76.5 % CO₂ conversion. In terms of jet fuel energy consumption, the tail gas recycle process requires less energy for CO₂ conversion at 61.9 % and 76.5 % scenarios. Therefore, the economic evaluation should be carried out to provide further guidance.

On the other hand, when these two water removal approaches are compared with the base case in Fig. 10, it can be clearly found that the reduction of energy consumption for jet fuel regardless of the increase in total energy consumption. Moreover, it is found that the recycle system (90 % recycle) requires the lowest energy consumption for jet fuel (4.57 MW/t jet fuel) than other CO₂-FTS processes and achieves the highest CO₂ conversion (85.8 %). This superior performance is attributed to the 90 % tail gas recycle, which produces the highest jet fuel yield.

5. Economic analysis of the modified CO₂-FTS process for jet fuel production at commercial scale

5.1. Economic methodology

The economic analysis of the CO₂-FTS process was conducted using the Aspen Process Economic Analyzer® (APEA) and the detailed process

Table 10
Equipment installed cost breakdown for base case, multi-stage CO₂-FTS and CO₂-FTS with tail gas recycle.

Equipment	Base case		Multi-stage CO ₂ -FTS		Three-stage		CO ₂ -FTS with tail gas recycle 63.8 % recycle		80.3 % recycle		90 % recycle	
	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)	Equipment installed cost (M\$)
H ₂	57.61	57.61	57.61	57.61	57.61	57.61	57.61	57.61	57.61	57.61	57.61	57.61
compressor	13.14	13.14	13.14	13.14	13.14	13.14	13.14	13.14	13.14	13.14	13.14	13.14
CO ₂	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87	1.87
compressor	55.25	55.25	55.25	55.25	55.25	55.25	55.25	55.25	55.25	55.25	55.25	55.25
Heater	93.33	93.33	93.33	93.33	93.33	93.33	93.33	93.33	93.33	93.33	93.33	93.33
CO ₂ -FTS reactor	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23
Cooler	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17
Three-phase separator												

flowsheets are shown in Figs. 5–7. APEA calculates the purchased and installed equipment cost for CO₂-FTS process such as the compressors, heater, cooler, from which the total direct cost of the plant is calculated. CAPEX is derived from the total direct cost with the accounting of other financial items such as indirect cost, engineering and contingency. The OPEX consists of the fixed operating and maintenance costs (fixed OPEX) and the variable operating and maintenance costs (variable OPEX). The fixed OPEX assumed as 3 % of CAPEX is made up of the total maintenance cost, labour costs, administration cost, and other cost [34]. The variable OPEX is based on feedstock cost and utility cost obtained from the APEA with their unit price.

The financial parameters used in the economic evaluation are shown in Table 9. CO₂ is assumed to be free from a CO₂ capture plant [35]. The hydrogen price was assumed to be \$2/kg which is the 2025 target of renewable hydrogen from electrolysis [36]. Other parameters are commonly used for the economic evaluation of a commercial plant [25,34,37].

It is noted that the CO₂-FTS reactor cannot be mapped in APEA, therefore it was considered as zero cost. Alternatively, Eqs. (17) and (18) are used to calculate the equipment installed cost of the CO₂-FTS reactor, using an installation factor of 2.75 and a scaling exponent of 0.8. The base cost and base size are referred to Zang et al. [24].

$$\text{Equipment installed cost} = \text{Purchased equipment cost} \times \text{Installation factor} \quad (17)$$

$$\text{Purchased equipment cost} = \text{Base cost} \times \left(\frac{\text{New size}}{\text{Base size}} \right)^{\text{Scaling exponent}} \quad (18)$$

The annual capital cost (ACC) was calculated by annualizing the CAPEX using Eq. (19) with plant lifetime n , and interest rate i .

$$\text{ACC} = \text{CAPEX} \left(\frac{i(1+i)^n}{(1+i)^n - 1} \right) \quad (19)$$

The total annual cost shown in Eq. (20) is the sum of ACC and OPEX.

$$\text{Total annual cost} = \text{ACC} + \text{Fixed OPEX} + \text{Variable OPEX} \quad (20)$$

The MSP of jet fuel was obtained from the Eq. (21) [38].

$$\text{MSP} = \frac{\text{Total annual cost}}{\text{Operating time per year} \times Y_{\text{Jetfuel}}} \quad (21)$$

5.2. Economic evaluation results

The economic performance of the CO₂-FTS process was performed for base case, multi-stage CO₂-FTS, and CO₂-FTS with tail gas recycle process. The installed equipment costs in Table 10 were obtained from APEA. It is noticeable that compressors and CO₂-FTS reactors dominate the total equipment installed cost for different CO₂-FTS processes. The installed cost of the CO₂ compressor and H₂ compressor remain constant at 13.1 M\$ and 57.6 M\$ for all CO₂-FTS processes because the feedstock is only compressed initially and there is no pressure drop after gas compression. While the increase in equipment installed cost of the CO₂-FTS reactor can be seen for both water removal configurations. With the addition of more stages, the installed cost of the CO₂-FTS reactor is 93.3 M\$ for two stages process and 119.1 M\$ for three stages process. The increase in these costs is due to the addition of more reactors in the multi-stage process. For the tail gas recycle process, as the recycle ratio changes from 0 to 90 %, the installed cost of the CO₂-FTS reactor varies from 55.3 M\$ to 104.6 M\$ due to the larger reactor size required.

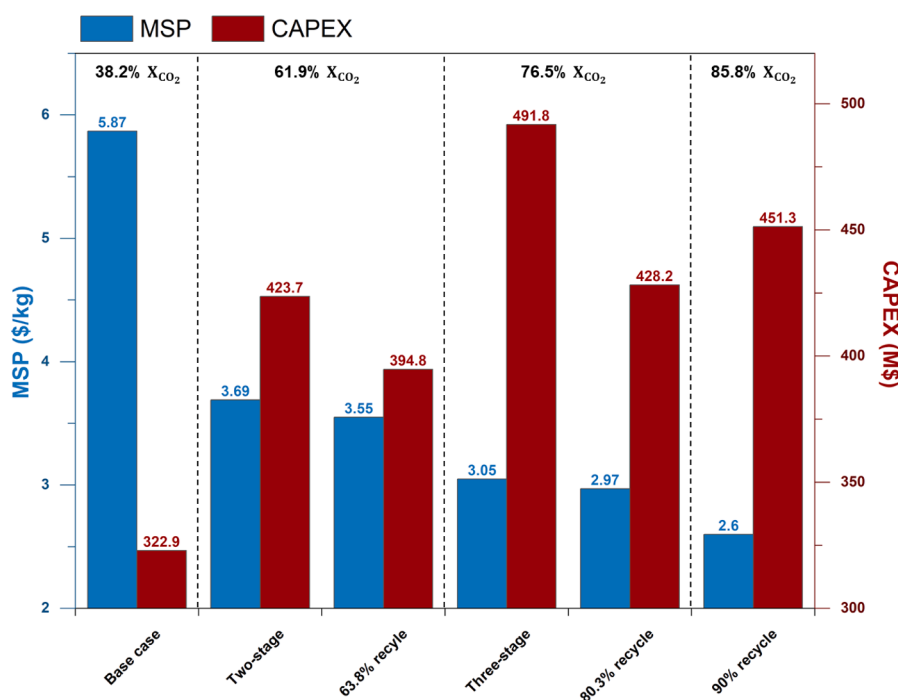
Table 11 presents the CAPEX breakdown and Table 12 summarises the economic performance. The best economic performance for jet fuel production is achieved by CO₂-FTS with 90 % tail gas recycle. This process can potentially reduce the MSP from \$5.87/kg to \$2.6/kg, which is only 44 % of the base case price. For comparison with current market

Table 11CAPEX breakdown for base case, multi-stage CO₂-FTS and CO₂-FTS with tail gas recycle.

Parameter			Base case	Multi-stage CO ₂ -FTS		CO ₂ -FTS with tail gas recycle		
				Two-stage	Three-stage	63.8 % recycle	80.3 % recycle	90 % recycle
TDC	Total direct cost (M\$)		128.27	168.33	195.38	156.85	170.11	179.28
TIC	Total indirect cost	20 % of TDC	25.65	33.67	39.08	31.37	34.02	35.86
BEC	Bare erected cost	TDC + TIC	153.93	202.00	234.46	188.22	204.13	215.14
EC	Engineering and contactor	27 % of BEC	41.56	54.54	63.30	50.82	55.12	58.09
EPC	Engineering procurement and construction	127 % of BEC	195.49	256.53	297.77	239.04	259.25	273.23
PC	Process contingency	25 % of BEC	38.48	50.50	58.62	47.06	51.03	53.79
PJC	Project contingency	20 % of EPC + 5 % of BEC	46.79	61.41	71.28	57.22	62.06	65.40
TPC	Total plant cost	120 % of EPC + 30 % of BEC	280.77	368.44	427.66	343.32	372.34	392.42
OC	Owner's cost	15 % of TPC	42.11	55.27	64.15	51.50	55.85	58.86
CAPEX	Total capital expenditure	115 % of TPC	322.88	423.71	491.81	394.82	428.19	451.28

Table 12Summary of the economic evaluation of base case, multi-stage CO₂-FTS and CO₂-FTS with tail gas recycle.

Description			Base case	Multi-stage CO ₂ -FTS		CO ₂ -FTS with tail gas recycle		
				Two-stage	Three-stage	63.8 % recycle	80.3 % recycle	90 % recycle
CAPEX (M\$)			322.88	423.71	491.81	394.82	428.19	451.28
ACC (M\$/yr)			37.93	49.77	57.77	46.37	50.30	53.01
Fixed OPEX (M\$/yr)			9.69	12.71	14.75	11.84	12.85	13.54
Variable OPEX (M\$/yr)	Utility cost	Electricity	16.38	16.38	16.38	16.38	16.38	16.38
		Cooling water	0.61	0.91	1.09	0.93	1.07	1.18
		Heating	2.92	4.70	5.76	4.47	5.46	5.69
	Feedstock cost	CO ₂	0.00	0.00	0.00	0.00	0.00	0.00
		H ₂	241.92	241.92	241.92	241.92	241.92	241.92
Total annual cost (M\$/yr)			309.44	326.39	337.67	321.92	327.97	331.71
Minimum selling price of jet fuel (\$/kg)			5.87	3.69	3.05	3.55	2.97	2.60

**Fig. 11.** Summary of MSP and CAPEX for different CO₂-FTS process.

in 2022 [39], this is 2.4 times higher than the average market price of conventional jet fuel (\$1.1/kg), while it is only slightly higher than the SAF price in 2022 (\$2.4/kg). The three-stage CO₂-FTS process was found to have the worst economic performance in terms of CAPEX and total annual cost. It is worth noting that the feedstock cost of hydrogen is the largest contributor to the total annual cost and MSP. For the base case

process, 78 % of the total annual cost comes from hydrogen costs. This is consistent with the previous study for the production of fuel based on CO₂ and hydrogen [24]. Therefore, for reducing the MSP of jet fuel, the main goal is to investigate how to reduce the price of hydrogen.

5.3. Comparison between two ex-situ water removal configurations

Two ex-situ water removal configurations were compared at the same CO₂ conversion level (61.9 % and 76.5 %) for total cost and produced fuel cost. To clearly indicate the total cost for different process, the CAPEX was used for comparison instead of total annual cost. This is because the hydrogen demand is same for different process while hydrogen cost accounts roughly three quarters of total annual cost (Table 12). The economic analysis results shown in Fig. 11 indicate that the tail gas recycle process has lower CAPEX and MSP of jet fuel compared to the multi-stage process at the same CO₂ conversion. For 61.9 % CO₂ conversion case, the CAPEX is reduced from 423.7 to 394.8 M\$, and the MSP is reduced from 3.69 to 3.55 \$/kg. For 76.5 % CO₂ conversion, these values are from 491.8 to 428.2 for CAPEX and from 3.05 to 2.97 for MSP. Surprisingly, the CAPEX for the 90 % tail gas recycling process is 451.3 M\$, which is even lower than 491.8 M\$ for the three-stage process. This means that the 90 % tail gas recycling process can achieve higher CO₂ conversion (85.8 %), but with lower invested CAPEX. From an economic point of view, the CO₂-FTS process with tail gas recycle can save costs compared to the multi-stage CO₂-FTS process.

6. Conclusion

In this study, a CO₂-FTS model for jet fuel production was developed in Aspen Plus® linked to ACM. The model was validated at the lab scale using experimental ASF plots and hydrocarbon selectivity. Technical analysis was conducted to predict the performance improvement of the commercial CO₂-FTS process through two ex-situ water removal configurations. Compared to the base case scenario, the three-stage CO₂-FTS process achieved a doubling (100 % increase) in both CO₂ conversion and jet fuel yield. In the CO₂-FTS process with a 90 % tail gas recycle, CO₂ conversion and jet fuel yield increased by 124 % and 107 %, respectively. Although the highest total energy demand was identified for CO₂-FTS with 90 % tail gas recycle (260 MW), this system has the lowest unit energy demand (4.57 MWh per ton of jet fuel) due to the highest jet fuel productivity. For the same level of CO₂ conversion, the multi-stage CO₂-FTS behaves almost identically to the CO₂-FTS with tail gas recycle. Further indications from the economic analysis show that the tail gas recycle has lower CAPEX and MSP costs due to the use of less equipment compared to the multi-stage CO₂-FTS process. In conclusion, CO₂-FTS with a high tail gas recycle rate has the potential to improve the performance of commercial CO₂ utilisation plants from both technical and economic point of views.

CRedit authorship contribution statement

Yide Han: Writing – original draft, Validation, Software, Methodology, Formal analysis, Conceptualization. **Ariane D.N. Kamkeng:** Writing – review & editing, Validation, Software, Methodology. **Olajide Otitoju:** Writing – review & editing. **Yuxing Ding:** Writing – review & editing. **Meihong Wang:** Writing – review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors would like to acknowledge the financial support of the EU RISE project OPTIMAL (Grant Agreement No: 101007963).

Data availability

Data will be made available on request.

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