

Full Length Article

Yield optimization of power-to-liquid kerosene via Fischer-Tropsch synthesis

Mohammed Owais Khokar^{a,*}, Simil Shajan^a, Simon Maier^{a,b}, Nathanael Heimann^a, Ralph-Uwe Dietrich^a

^a German Aerospace Center, Institute of Engineering Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany

^b Since 01 January 2026, German Aerospace Center, Institute of Future Fuels, Linder Höhe, 51147 Köln, Germany

ARTICLE INFO

Keywords:

Power-to-liquid
Fischer-Tropsch
Kerosene production
Sustainable aviation fuel
Aspen Plus®

ABSTRACT

Sustainable aviation fuels (SAFs) are considered a key enabler for reducing aviation greenhouse gas emissions and supporting long-term climate neutrality targets. Among approved pathways, the Power-to-Liquid (PtL) pathway via Fischer-Tropsch (FT) synthesis offers a scalable route to convert renewable electricity and CO₂ into drop-in aviation fuels. However, FT synthesis produces a broad hydrocarbon spectrum, necessitating extensive downstream upgrading to maximize kerosene yield and meet ASTM D7566 specifications. This can be achieved by optimizing both the FT synthesis and the hydrocracker operating conditions. Previous studies have primarily focused on individual process steps or on alternative process configurations, limiting the identification of their combined impact on kerosene production. This study presents an integrated techno-economic assessment of PtL FT kerosene production using a coupled Aspen Plus®-Python simulation framework. The simulation model incorporates validated Python-based kinetic models for FT synthesis and hydrocracking within a PtL process chain, enabling a systematic evaluation of their influence on kerosene yield, process efficiencies and production costs. The results show that optimization enables a kerosene yield of 87.6 % and a kerosene carbon efficiency of 86.9 %. Despite the high kerosene yield, the process remains energy intensive, exhibiting a Power-to-kerosene efficiency of 34.8 % and a net production cost (NPC) of 7.0 €₂₀₂₄ kg_{kerosene}⁻¹, dominated by electricity consumption (45–58 %). The analysis reveals that maximizing kerosene yield does not inherently minimize the production cost. By-product revenues from e-gasoline and e-diesel can reduce the NPC to 6.2 €₂₀₂₄ kg_{kerosene}⁻¹. Consequently, commercial viability increasingly depends on the market value of by-products.

1. Introduction

The decarbonization of the aviation sector remains a major challenge, as direct electrification and hydrogen-based propulsion systems are currently limited by technological and operational constraints. Within the framework of the European Green Deal, the European Union aims to reduce the greenhouse gas emissions in the transport sector by

90 % by 2050 [1], while aviation demand is projected to increase significantly. According to the European Aviation Environmental Report 2025 [2], the annual traffic growth in the EU27 + EFTA region is projected to increase from 8.35 million in 2023 to 13.8 million flights by 2050 under the high-growth scenario. Under the corresponding scenario, annual CO₂ emissions are projected to reach approximately 228 million tons, thereby intensifying the need for scalable and effective mitigation strategies.

Abbreviations: ACC, Annual capital cost; MtJ, Methanol-to-Jet; ASF, Anderson-Schulz-Flory; NPC, Net production cost; ASTM, American Society for Testing and Materials; OPEX_{dir}, Direct operational expenditures; BioCCS, Bioenergy with carbon capture and storage; OPEX_{ind}, Indirect operational expenditures; BtL, Biomass-to-liquid; PBtL, Process-biomass-to-liquid; CAPEX, Capital expenditures; PEM, Proton exchange membrane; CEPCI, Chemical Engineering Plant Cost Index; PR-BM, Peng-Robinson with Boston-Mathias modifications; DLR, Deutsches Zentrum für Luft- und Raumfahrt; PtL, Power-to-liquid; EC, Equipment cost; PyTEEA, Python-based tool for techno-economic and environmental assessment; FCI, Fixed capital investment; ReFuelEU, European Union initiative for sustainable aviation fuels in aviation; FT, Fischer-Tropsch; RFNBO, Renewable fuels of non-biological origin; FT-SPK, Fischer-Tropsch synthetic kerosene; RWGS, Reverse water gas shift; SPK/A, Synthetic kerosene with aromatics; SAF, Sustainable aviation fuel; HC, Hydrocracker; SBCR, Slurry bubble column reactor; HEFA, Hydro-processed esters and fatty acids; TCI, Total capital investment; HT, Hydrotreater; VLE, Vapor-liquid equilibrium; IR, Interest rate; WHSV, Weight hourly space velocity; LHHW, Langmuir-Hinshelwood-Hougen-Watson.

* Corresponding author.

E-mail address: owais.khokar@dlr.de (M.O. Khokar).

<https://doi.org/10.1016/j.fuel.2026.141247>

Received 23 June 2026; Received in revised form 9 August 2026; Accepted 2 September 2026

Available online 8 September 2026

0016-2361/© 2026 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Nomenclature		
Symbols		
Symbol	Description & Unit	
DENOM	Coverage term for vacant primary FTS sites –	
DENOM*	Coverage term for vacant secondary sites –	
f_{H_2}	Fugacity of hydrogen Pa	
f_{iso}	Fugacity of iso-paraffin Pa	
f_n	Fugacity of paraffin Pa	
k	Reaction rate constant Unit dependent	
k^*	Secondary reaction rate constant Unit dependent	
k_M^*	Lumped secondary methane formation rate constant mol·(g _{cat} ·h·MPa ²) ⁻¹	
K	Equilibrium constant for FT synthesis Unit dependent	
K^*	Secondary equilibrium constant Unit dependent	
k_{cr}	Rate constant for cracking reaction of iso-paraffin (kmol/h)·kg _{cat} ⁻¹	
k_{eq}	Equilibrium constant for cracking and isomerization (kmol/h)·kg _{cat} ⁻¹	
k_{isom}	Rate constant for isomerization reaction of paraffin (kmol/h)·kg _{cat} ⁻¹	
$K_{L,iso}$	Langmuir adsorption constant for iso-paraffin MPa ⁻¹	
$K_{L,n}$	Langmuir adsorption constant for paraffin MPa ⁻¹	
K_{PD}	Product of the protonation and dehydrogenation constants MPa ⁻¹	
LHV _{H₂}	Lower heating value of hydrogen MWh·kg ⁻¹	
LHV _{kerosene}	Lower heating value of kerosene MWh·kg ⁻¹	
n	Number of carbon atoms –	
n_i	Number of moles of component I mol	
$n_{i,new}$	New mole amount of component I mol	
$n_{i,updated}$	Updated mole amount of component I mol	
P	Total operating pressure bar	
P_{CO}	Partial pressure of CO MPa	
P_{el}	Electrical power demand MW	
P_{FT}	FT reactor operating pressure bar	
P_{H_2}	Partial pressure of H ₂ MPa	
P_{H_2O}	Partial pressure of H ₂ O MPa	
P_{HC}	HC operating pressure MPa	
r_{cr}	Reaction rate for cracking of iso-paraffin kmol·(kg/h) ⁻¹	
r_{isom}	Reaction rate for isomerization of n-paraffin into iso-paraffin kmol·(kg/h) ⁻¹	
$r_{prod,iso}$	Formation rate of iso-paraffin kmol·(kg/h) ⁻¹	
$r_{prod,n}$	Formation rate of n-paraffin kmol·(kg/h) ⁻¹	
r_{cr}	Reaction rate for cracking of iso-paraffin kmol·(kg/h) ⁻¹	
$R_{C_nH_{2n}}$	Overall 1-olefin formation rate mol·(g _{cat} ·h) ⁻¹	
$R_{C_nH_{2n+2}}$	Overall n-paraffin formation rate mol·(g _{cat} ·h) ⁻¹	
R_{CH_4}	Methane formation rate mol·(g _{cat} ·h) ⁻¹	
$R_{C_nH_{2n}}^{*,hydrogenation}$	Secondary olefin hydrogenation rate mol·(g _{cat} ·h) ⁻¹	
$R_{C_nH_{2n}}^{primary}$	Primary olefin formation rate mol·(g _{cat} ·h) ⁻¹	
$R_{C_nH_{2n+2}}^{primary}$	Primary paraffin formation rate mol·(g _{cat} ·h) ⁻¹	
$R_{CH_4}^{primary}$	Primary methane formation rate mol·(g _{cat} ·h) ⁻¹	
$R_{CH_4}^{secondary}$	Secondary methane formation rate mol·(g _{cat} ·h) ⁻¹	
T	Temperature °C	
T_{FT}	FT reactor operating temperature °C	
T_{HC}	HC operating temperature °C	
X_{CO}	Overall CO conversion %	
$X_{CO,i}$	CO conversion into component I %	
$Y_{component,i}$	Yield of component I %	
Greek symbols		
Symbol	Description&Unit	
α	ASF growth probability factor –	
α_n	ASF growth probability for chain with n carbon atoms –	
η_{H_2tk}	Hydrogen-to-kerosene efficiency %	
η_{ptk}	Power-to-kerosene efficiency %	
$\dot{m}_{HC,new}$	New HC recycle stream mass flow rate kg·h ⁻¹	
$\dot{m}_{HC,old}$	Initial HC recycle stream mass flow rate kg·h ⁻¹	
$\dot{m}_{HC,updated}$	Updated HC recycle stream mass flow rate kg·h ⁻¹	
$\dot{m}_{kerosene}$	Kerosene production mass flow rate kg·h ⁻¹	
$\dot{m}_{REC,new}$	New recycle stream mass flow rate kg·h ⁻¹	
$\dot{m}_{REC,old}$	Initial recycle stream mass flow rate kg·h ⁻¹	
$\dot{m}_{REC,updated}$	Updated recycle stream mass flow rate kg·h ⁻¹	
τ	Total residence time kg _{cat} ·(kg _{wax} , IN/h) ⁻¹	

Sustainable aviation fuel (SAF) is anticipated to play a central role in the future of environmentally sustainable aviation. It has the potential to contribute around 65 % of the emissions reduction required for the aviation to reach net zero CO₂ emission by 2050. This contribution is attributed to the lower life-cycle greenhouse gas emissions of SAF compared with conventional jet fuel [3]. To accelerate the deployment in the EU, the ReFuelEU Aviation Regulation mandates a progressive increase in the minimum share of SAF in the aviation fuel made available to aircraft operators at airports within the scope of the Regulation. The required share increases from 2 vol% in 2025 to 70 vol% by 2050, including a dedicated minimum share for synthetic aviation fuels (RFNBOs) that reaches 35 vol% by 2050 [4]. Among the American Society for Testing and Materials (ASTM) approved SAF production pathways, Power-to-liquid (PtL) offers a promising and scalable solution by converting CO₂ and renewable H₂ into synthetic hydrocarbons, thereby avoiding the limitations associated with the biomass availability and land use constraints. Despite its potential, PtL-based SAF possess key challenges related to process efficiency, product selectivity and economic viability. A key limitation arises from the Fischer-Tropsch (FT) synthesis, which produces a wide spectrum of hydrocarbons. As a result, only a fraction of a product lies within the desired kerosene-range, while significant quantities of byproducts such as gasoline, diesel and heavy waxes are produced, necessitating extensive downstream upgrading. These upgrading processes are essential to meet the fuel quality

requirements defined by ASTM D7566 [5].

Previous work has investigated the PtL process chain with varying scope and detail, and their contributions provide important context for the present work. Adelung et al. [6] focused on the detailed simulation and cost estimation of the FT-based PtL process, including an allothermal reverse water gas shift reactor (RWGS) reactor with heat supply from an oxyfuel burner, a FT synthesis based on Anderson-Schulz-Flory (ASF) mechanism, and a simplified hydrocracker (HC) model. Their study identified optimal operating conditions for maximizing carbon, hydrogen and PtL efficiency. Furthermore, they suggested operating the RWGS reactor at elevated temperature of 825 °C and a moderate pressure of 5 bar to improve efficiency while avoiding carbon formation, potentially contributing to lower product costs. Habermeyer et al. [7] developed a detailed simulation of FT synthesis for the Power-Biomass-to-Liquid (PBtL) pathway, incorporating the FT kinetic model using the reaction kinetics proposed by Todici et al. [8] and examined the influence of CO₂ recycle and H₂/CO ratio on the carbon efficiency and the production cost of liquid hydrocarbons.

Several recent studies have focused either on detailed kinetic modelling of FT synthesis, or on comparing different process configurations and technologies. For instance, Ostadi et al. [9] implemented three FT kinetic models representing cobalt catalysts with different support materials, including the simplified kinetic model proposed by Todici et al. [8]. They investigated the influence of H₂/CO ratio on the FT

synthesis performance in the context of a biomass-to-liquid (BtL). Their results demonstrated that the H_2/CO ratio has a significant influence on the hydrocarbon production rates, H_2 consumption and carbon efficiency, with an optimal ratio below 2. While the study provided insights into the influence of syngas composition on the hydrocarbon selectivity at the FT reactor outlet, the effects of the operating parameters, including reaction temperature and pressure, were not evaluated. Eyberg et al. [10] conducted a techno-economic assessment of FT and Methanol-to-Jet processes (MtJ) via the PtL pathway, evaluating multiple process configurations in Aspen Plus®. However, their assessment did not include a detailed upgrading of the syncrude, which limits the completeness of SAF production chain analysis and the conclusions that can be drawn regarding final fuel quality and kerosene yield. Kirsch et al. [11] studied two FT process configurations and systematically evaluated the influence of the FT reactor temperature and weight hourly space velocity (WHSV), as well as the effect of wax and tail gas recycling, on C_{10} - C_{20} selectivity at a constant operating pressure of 30 bar. Their results showed that gas recycling substantially improves liquid fuel yield, while wax recycling provides a modest improvement in C_{10} - C_{20} selectivity of up to 6 %. However, the effect of varying H_2/CO feed ratio on FT synthesis is not examined, and the definition of the kerosene range product relied on a generalized carbon number cut (C_{10} - C_{20}) rather than boiling point cuts, which are relevant when assessing hydrocracker performance and recycle strategies. Bube et al. [12] compared the FT and MtJ pathways over the complete PtL chain, reporting the kerosene output as a carbon efficiency relative to the CO_2 feed, and obtained a lower kerosene efficiency for the FT pathway (72 %) than for the MtJ pathway (76 %) in their reference cases. However, this comparison is based on a fixed FT chain growth probability and a fixed carbon number cut, without considering the joint optimization of the FT synthesis and HC operating conditions. As a result, the attainable carbon efficiency for the FT pathway is correspondingly limited. A structured comparison of these studies with the present work, covering the modelling approaches, the defined operating boundary, the kerosene fraction definition, the compliance with kerosene specifications, and the techno-economic scope, is presented in Table 1.

Overall, these studies tend to focus either on isolated process steps, kinetic modelling, or on comparisons across different process configurations. As a result, they do not fully exploit how the broad product spectrum from FT synthesis can be maximized toward specific kerosene-range hydrocarbons through downstream upgrading. This limitation is important because kerosene yield and fuel quality are not determined by FT synthesis alone, but by the interaction between the synthesis conditions and the upgrading severity. Without considering this interaction, it is difficult to identify operating conditions that maximize kerosene yield while simultaneously meeting fuel specifications and maintaining favorable economic performance. Furthermore, this limitation in the integration of the FT synthesis and upgrading process contributes to the

comparatively low kerosene yield and carbon efficiency reported for the FT pathway relative to the MtJ pathway in the literature.

To address this gap, this study investigates how FT synthesis conditions and HC operation can jointly increase kerosene yield. A detailed process simulation of the complete kerosene production process chain via PtL pathway is simulated. The process encompasses hydrogen production via electrolysis, syngas generation in an electrically operated RWGS, hydrocarbons synthesis using the FT kinetic model of Todici et al. [8], and hydrocarbon upgrading using the HC kinetic model of Gambaro et al. [13]. The process flowsheet was adapted from the Adelung et al. [6] with relevant modifications. The primary objectives are to:

- elucidate how FT and HC operating conditions individually and jointly influence kerosene yield.
- identify operating conditions that maximize the kerosene yield while meeting the key SAF-quality specifications.
- assess the economic viability of product composition, including the balance between kerosene, gasoline, and diesel. The kerosene stream is benchmarked against the ASTM D7566 specifications.

2. Process description

This section presents the modelling and simulation framework and fundamental assumptions underlying the PtL FT process, covering each individual process step from syngas conversion through to product separation and kerosene quality assessment.

2.1. General modelling assumptions

The PtL kerosene production is simulated using Aspen Plus® V14. The equation of state Peng-Robinson with Boston-Mathias modifications (PR-BM) is used, which is recommended for oil and gas as well as hydrocarbon separation [14]. Chemical species involved in the process model are H_2 , CO , CO_2 , H_2O , N_2 , O_2 , alkanes (C_1 - C_{30}), alkenes (C_1 - C_{30}) and iso-alkanes (C_1 - C_{30}). C_{30+} components are not explicitly modelled to reduce the model complexity and are instead represented by C_{30} , as they exhibit similar thermodynamic behavior. Furthermore, alcohols, aromatics, and cyclic components are not included, as the kinetic model from Todici et al. [8] does not predict the formation of these species. The process flowsheet is shown in Fig. 1. The plant is sized based on an exemplary 100 MW_{el} proton exchange membrane (PEM) electrolyser, which produces H_2 at a rate of 1.8 t_{H₂}/h at an overall efficiency of 60 %_{LHV}. The operating condition of PEM is set to 80 °C and 30 bar [15]. The required CO_2 for the synthesis is assumed to be available and stored at −30 °C and 15 bar.

Table 1

Overview of the FT and HC modelling approaches, operating boundaries, and analysis scope in previous studies and the present work.

Study	Kinetic model	Operating boundary	Kerosene fraction definition	Kerosene-spec compliance	TEA scope
Ostadi et al. [9]	Three cobalt-based FT kinetic models; HC kinetic not included	FT synthesis only; effect of H_2/CO ratio studied	Hydrocarbon selectivity after FT reactor	Not addressed	Not included
Eyberg et al. [10]	Lumped FT macro-kinetic ASF model, olefins = 8 % of paraffins; HC kinetics not included	Different process configurations	C_8 - C_{16} carbon cut	Qualitative	Full TEA (LCOP)
Kirsch et al. [11]	Detailed FT kinetic model (alkanes only, olefins not resolved); HC from Gambaro et al. [13] with Sun parameters	Coupled FT-HC configurations; FT CO conversion; HC: WHSV, Temperature variation studied, H_2/CO ratio and pressure fixed	C_{10} - C_{20} carbon lump	Not addressed	Not included
Bube et al. [12]	ASF model, fixed chain growth probability (0.85); fixed cracking	Comparison of FT and MtJ technologies	C_8 - C_{16} carbon cut	Qualitative	Technical only
This study	FT kinetic model from Todici et al. [8] (paraffins and olefins); detailed HC kinetic model from Gambaro et al. [13]	Coupled FT-HC process configuration; FT (T , H_2/CO) and HC (T , P , WHSV) studied simultaneously	Boiling-point cut	Benchmarked vs ASTM D7566 (A1/A2)	Full TEA (NPC)

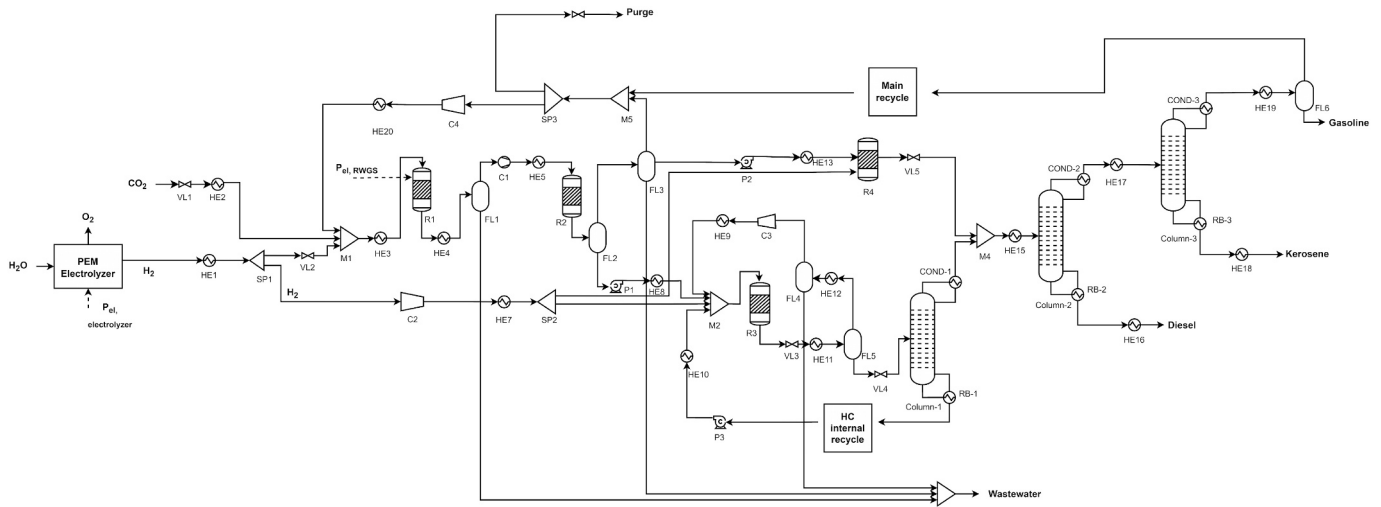


Fig. 1. Process flow diagram of PtL-Kerosene production via Fischer-Tropsch route.

2.2. Reverse water gas shift reaction

The H_2 stream is heated to 225 °C and split into two streams, one is fed to the RWGS reactor (R1), and the other stream is directed to the HC unit. The required CO_2 flow is fixed based on the H_2/CO molar ratio required for the FT synthesis. Both H_2 and CO_2 streams, along with the recycle stream, are conditioned to the operating condition of RWGS reactor of 825 °C and 5 bar [16]. The RWGS reactor is modelled as a Gibbs reactor (Gibbs minimization). The produced wet syngas stream is subsequently cooled in flash drum (FL1) to separate most of the co-produced water, in order to prevent the catalyst deactivation in the downstream FT synthesis. The overhead vapor from the flash drum constitutes dried syngas (4 mol%), which is then fed to the FT synthesis step.

2.3. Fischer-Tropsch synthesis

The dried syngas is compressed to the operating condition of FT reactor i.e. 25 bar using a multi-stage compressors (C1) before being fed to the FT reactor (R2). The FT reactor is considered as the slurry bubble column reactor (SBCR) and the intrinsic kinetic model proposed by Todici et al. [8], which was experimentally validated using a catalyst (Co-Re/ Al_2O_3), is employed. The selection of the FT catalyst depends on the operating conditions, syngas composition, and desired hydrocarbon range. Cobalt-based catalysts are the preferred industrial catalysts for low temperature FT synthesis because of their high activity, low water gas shift activity, high selectivity toward long chain paraffinic hydrocarbons [17]. Rhenium is well-established promoter that enhances cobalt reducibility and metal dispersion, thereby improving catalytic activity [18]. Furthermore, commercial low temperature FT plant also employ Cobalt based catalyst (Co- Al_2O_3), for e.g. the Sasol slurry bed plant at Ras Laffan, Qatar [17]. Although, the composition of commercial FT catalysts are proprietary, promoted cobalt catalysts supported on Al_2O_3 are widely used in the literature [7,8,19,20]. At a large scale plant, SBCR has an advantage of its low investment costs in comparison to micro-channel reactors [20,21] and its high CO conversion per pass compared to fixed bed reactors [20,22]. The FT reactor is simulated as a RSTOIC model, with the external Python-based reaction kinetic model as proposed in Todici et al. [8], see Section 2.7.1. This kinetic model is based on Langmuir Hinshelwood Hougen Watson (LHHW) and considers both primary and secondary reactions as well as secondary 1-olefin hydrogenation occurring on the catalyst sites. The terms ‘primary’ and ‘secondary’ refers to the formation of paraffins, olefins, methane, and ethene on the primary and secondary sites of the catalyst, respectively. The reaction rate equations, eq. 1–11, are listed below. Further reactions

rate equations as well as value for constants can be found in SI chapter A.1.

$$R_{C_nH_{2n+2}}^{primary} = k_7 K_2^{0.5} P_{H_2}^{0.5} \alpha_1 \alpha_2 \prod_{i=3}^n \frac{\alpha_i}{DENOM^2} \quad n \geq 2 \quad (1)$$

$$R_{C_nH_{2n}}^{primary} = k_{8,0} e^{c_n} \alpha_1 \alpha_2 \prod_{i=3}^n \frac{\alpha_i}{DENOM} \quad n \geq 3 \quad (2)$$

$$R_{C_2H_4}^{primary} = k_{8E} e^{c_2} \alpha_1 \frac{\alpha_2}{DENOM} \quad (3)$$

$$R_{CH_4}^{primary} = k_7 K_2^{0.5} P_{H_2}^{0.5} \frac{\alpha_1}{DENOM^2} \quad (4)$$

$$R_{CH_4}^{secondary} = \frac{k_M^* P_{CO} P_{H_2}}{DENOM^{*2}} \quad (5)$$

$$R_{C_nH_{2n}}^{*hydrogenation} = k_{OH} P_{C_nH_{2n}} K_2^* \frac{P_{H_2}}{DENOM^{*2}} \quad n \geq 2 \quad (6)$$

$$R_{C_nH_{2n+2}} = R_{C_nH_{2n+2}}^{primary} + R_{C_nH_{2n}}^{*hydrogenation} \quad n \geq 2 \quad (7)$$

$$R_{C_nH_{2n}} = R_{C_nH_{2n}}^{primary} - R_{C_nH_{2n}}^{*hydrogenation} \quad n \geq 2 \quad (8)$$

$$R_{CH_4} = R_{CH_4}^{primary} + R_{CH_4}^{secondary} \quad (9)$$

$$DENOM = 1 + K_1 P_{CO} + \sqrt{K_2 P_{H_2}} + \left(\frac{1}{K_2^* K_4 K_5 K_2} \cdot \frac{P_{H_2O}}{P_{H_2}^{0.5}} + \sqrt{K_2 P_{H_2}} \right) \cdot (\alpha_1 + \alpha_1 \alpha_2 + \alpha_1 \alpha_2 \sum_{j=3}^{30} \prod_{j=3}^i \alpha_j) \quad (10)$$

$$DENOM^* = 1 + k_1^* P_{CO} + \sqrt{k_2^* P_{H_2}} + \left(\frac{1}{k_5^* K_2^{*0.5}} \cdot \frac{P_{H_2O}}{P_{H_2}^{0.5}} \right) \quad (11)$$

In the kinetic expressions, k_i and K_i denote the reaction rate constant and equilibrium constant of reaction i , respectively. For instance, k_{8E} represents the reaction rate constant associated with the rate determining step for reaction (8), which describes the methane formation on secondary active sites. Furthermore, α_i represents the chain growth probability factor, R_i represents the reaction rate of species i , and P_i denotes the partial pressure of component i . Eqs. (1)–(4) describes the rate expressions for the primary FT reactions and the methane formation on

secondary catalyst sites is represented by Eq. (5). Moreover, olefin hydrogenation to paraffins is also incorporated in the model and described by Eq. (6). Eqs. (7)–(9) defines the overall formation rates of hydrocarbons by accounting for both primary and secondary FT reactions. The terms DENOM and DENOM* represents the LHHW adsorption denominator, accounting for the surface coverage and competitive adsorption of reacting species on the primary and secondary catalytic sites. For each hydrocarbon, a reaction rate is determined by its corresponding α and the fraction of vacant catalyst sites, which in turn is a function of the respective cumulative chain growth probabilities in the model. This α is expressed using Eqs. (12)–(14).

$$\alpha_1 = \frac{k_3 K_1 P_{CO}}{k_3 K_1 P_{CO} + k_7 \sqrt{K_2 P_{H_2}}} \quad (12)$$

$$\alpha_2 = \frac{k_3 K_1 P_{CO} [S]}{k_3 K_1 P_{CO} [S] + k_7 \sqrt{K_2 P_{H_2}} [S] + k_{8,0} e^{c \cdot n}} \quad (13)$$

$$\alpha_n = \frac{k_3 K_1 P_{CO} [S]}{k_3 K_1 P_{CO} [S] + k_7 \sqrt{K_2 P_{H_2}} [S] + k_{8,0} e^{c \cdot n}} n \geq 3 \quad (14)$$

Where, $\alpha_1, \alpha_2, \alpha_n$ represents the chain growth probabilities. P_{CO} and P_{H_2} are the partial pressures of the CO and H_2 , and S is the catalyst vacant site. Furthermore, k_i and K_i are the rate constants and equilibrium constants, respectively. The rate constants and equilibrium constants equation can be found in SI Note A.1. Furthermore, α is governed by the competition between propagation, driven by adsorbed CO [$k_3 K_1 P_{CO}$], and termination, driven by hydrogen [$k_7 \sqrt{K_2 P_{H_2}}$] and by temperature-activated 1-olefin desorption [$k_{8,0} e^{c \cdot n}$]. Owing to the complexity of this kinetic formulation, the reaction model was implemented as a FORTRAN user Kinetic subroutine, as documented in [23]. In the present study, the same model is reimplemented in Python, as described in Section 2.7. Although, Aspen Plus® supports the implementation of external reaction kinetics through FORTRAN user Kinetic subroutine. However, this approach requires additional Fortran compiler setup and provides limited transparency during computation. In contrast, Python-based implementation offers greater flexibility for model development and debugging, while enabling the flexible integration with the process simulation framework. This approach improves model transparency and facilitates rapid parameter studies without requiring the modification in the simulation. As illustrated in Table 2, four operating configurations were considered for the FT reactor at a fixed pressure of 25 bar [23], considering reaction temperatures of 220 °C and 230 °C and H_2/CO molar ratios of 1.6 and 2. The overall CO conversion was assumed to be 55 %, consistent with value reported in the [20], for a single-stage SBCR reactor operated with cobalt catalyst.

2.4. Upgrading of FT products

The hydrocarbons produced in the FT reactor, including paraffins and olefins, are sent through the series of flash separators (FL2, FL3). In the first flash stage (FL2), heavier hydrocarbons (C_{20+}) are separated at 150 °C and 25 bar and sent to a HC (R3) to increase the product yield toward kerosene. Subsequently, the second flash stage (FL3) is simulated as a three-phase separator, in which gas phase is recycled to the RWGS reactor, the aqueous phase water is removed and the light liquid hydrocarbons are sent to the hydrotreater reactor (HT, R4), where olefins are hydrogenated to stable paraffins in order to meet ASTM D7566

Table 2
Selected operating condition for FT synthesis.

Parameters	Unit	Selected values
Temperature	°C	220, 230
H_2/CO molar ratio	–	1.6, 2
CO conversion	%	55

specifications. The required H_2 for cracking and hydrogenation is determined based on the H_2/wax ratio and H_2/C ratio, respectively, and is supplied directly from the electrolyser to the reactors as shown in Fig. 1. HT reactor (R4) is modeled as RSTOIC reactor, where olefins are hydrogenated to paraffins in the presence of H_2 at 369 °C and 35 bar. HC reactor is modelled as a yield reactor, with the external Python-based reaction kinetic model developed by Gambaro et al. [13], see Section 2.7.2. This model based on the LHHW approach and provides the reaction network as mentioned in Eqs. (15)–(29).

$$\frac{dn_{isoC}(i)}{d\tau} = r_{isom}(i) + r_{prod,iso}(i) - r_{cr}(i) i = 6, 30 \quad (15)$$

$$\frac{dn_{isoC}(i)}{d\tau} = -r_{isom}(i) + r_{prod,iso}(i) i = 5 \quad (16)$$

$$\frac{dn_{isoC}(i)}{d\tau} = r_{prod,iso}(i) i = 4 \quad (17)$$

$$\frac{dn_{nC}(i)}{d\tau} = r_{isom}(i) + r_{prod,n}(i) i = 6, 30 \quad (18)$$

$$\frac{dn_{nC}(i)}{d\tau} = r_{isom}(i) + r_{prod,n}(i) + \frac{2}{5} r_{cr}(i+1) i = 5 \quad (19)$$

$$\frac{dn_{nC}(i)}{d\tau} = r_{prod,n}(i) + \frac{2}{5} r_{cr}(6) i = 3, 4 \quad (20)$$

$$\frac{dn_{nC}(i)}{d\tau} = \frac{2}{5} r_{cr}(6) i = 1, 2 \quad (21)$$

$$\frac{dn_{H_2}}{d\tau} = \sum_{i=6}^{30} r_{cr}(i) \quad (22)$$

$$r_{isom} = \frac{k_{isom}(i) \cdot (f_n(i) - \frac{f_{iso}(i)}{K_{eq}(i)})}{f_{H_2} \cdot [A] + B} \quad (23)$$

$$r_{cr} = \frac{k_{cr}(i) \cdot f_{iso}(i)}{f_{H_2} \cdot [A] + B} \quad (24)$$

$$r_{prod,iso}(i) = Par15 \cdot \sum_{j=i+4}^{30} \left(\frac{2}{j-6} r_{cr}(j) \right) + \frac{2}{2 \cdot (i+3) - 12} r_{cr}(i+3) \quad (25)$$

$$r_{prod,n}(i) = (1 - Par15) \cdot \sum_{j=i+4}^{30} \left(\frac{2}{j-6} r_{cr}(j) \right) \quad (26)$$

$$r_{prod}(i=3) = \sum_{j=7}^{30} \left(\frac{2}{2 \cdot (j) - 12} r_{cr}(j) \right) \quad (27)$$

$$A = 1 + \sum_{i=1}^{nC} f_n(i) \cdot K_{L,n}(i) + \sum_{i=4}^{nC} f_{iso}(i) \cdot K_{L,iso}(i) \quad (28)$$

$$B = K_{PD}(i) \cdot (K_{L,n}(i) \cdot f_n(i) + K_{L,iso}(i) \cdot f_{iso}(i)) \quad (29)$$

Eqs. (15)–(22) describes the formation of *iso*-paraffins and paraffins and consumption of hydrogen through isomerization and cracking reactions. The terms r_{isom}, r_{cr} denote the reaction rates of isomerization, and cracking, respectively, as mentioned in Eqs. (23)–(24), where the reaction rates depend on the adsorption equilibrium, hydrocarbon fugacity, hydrogen concentration and catalyst surface coverage. Furthermore, Eqs. (25)–(27), describe the redistribution of cracked fragments into *iso*- and *n*-paraffins with different carbon numbers, while Eqs. (28)–(29) define the adsorption terms and surface-site interactions governing the competitive adsorption behaviors of hydrocarbons on the catalyst active sites. Further kinetic expressions as well as constant values can be found in SI chapter A.2.

Similarly to the FT kinetic model, the HC kinetic model is also developed in Python. The detailed implementation of kinetic model is described in Section 2.7. Eight operating cases were defined to investigate the impact of HC operating conditions on kerosene yield. Table 3 summarize the selected operating parameters and their respective ranges. Furthermore, the cracking severity in the HC reactor is quantified using the wax conversion, as defined in Eq. (30), at the selected operating parameters [24]. The wax conversion defines the fraction of C_{22+} hydrocarbons cracked during one pass through the HC, thereby reflecting the cracking severity in relation to isomerization.

$$\text{waxconversion} = \frac{\omega_{C_{22+in}} - \omega_{C_{22+out}}}{\omega_{C_{22+in}}} \quad (30)$$

The cracked paraffins and iso-paraffins are first sent to a flash drum (FL5) to recover H_2 , which is recycled to the HC. The liquid fraction is sent to a distillation column (Column-1), where heavy paraffins and iso-paraffins are separated and recycled to the HC, while the light paraffins and iso-paraffins are sent to the final product separation. The specifications of the distillation column (Column-1) are optimized using design specification by varying the reflux ratio to achieve a mass recovery of the C_{17+} hydrocarbons to the HC reactor and thereby minimizing the diesel fraction in final product stream.

2.5. Product separation

The light hydrocarbons streams from both HT and HC reactors are mixed and sent to the final product separation. The final product separation consists of two distillation columns and a flash drum. In the first distillation column (Column-2), the heavier diesel fraction is separated from the mixture. The remaining stream is then sent to the second distillation column (Column-3), where the kerosene fraction is recovered. Subsequently, the lighter gasoline fraction is separated in the flash drum (FL6), while the remaining gases are recycled back to the RWGS unit. The internal design specifications of the distillation columns are defined to meet SAF quality requirements. Although a comprehensive quality assessment of the diesel and gasoline is important for commercial application, their compliance with relevant commercial fuel specifications and potential upgrading requirements are beyond the scope of this study. Therefore, a simplified quality assessment is performed. Specifically, Column-2 is optimized by adjusting the distillate-to-feed ratio to achieve a diesel flash point of 115 °C. This value is above the minimum flash point requirement specified for commercial diesel [25]. Column-3 is also optimized by varying the distillate-to-feed ratio to achieve a target kerosene flash point of 38 °C, as specified in ASTM D7566. Furthermore, FL6 is operated at −40 °C, which results in a gasoline fraction with a flash point of approximately −40.6 °C, which is consistent with reported flash point for commercial gasoline [26]. The design parameters of the distillation columns are provided in SI. Table A.4-A.6.

2.6. Product quality and specifications of SAF

The quality of the simulated kerosene is assessed based on key physicochemical properties relevant to blending specifications for mixing with conventional aviation fuel to ensure safe and reliable operation of aircraft. These requirements are governed by the standard ASTM D7566, which defines specifications for several approved synthetic blending pathways, including FT synthetic kerosene (FT-SPK) under

Table 3
Selected operating cases of HC reactor.

Parameters	Unit	Selected values
Temperature	°C	368, 373, 378
Pressure	Bar	35, 45, 55
WHSV	h ^{−1}	1, 1.5

Annex A1, hydro-processed esters and fatty acids (HEFA) under Annex A2 and synthetic kerosene with aromatics (SPK/A) under Annex A4 [3]. In this study, the kerosene stream obtained from the simulation is benchmarked primarily against the FT-SPK requirements to assess the extent to which the simulated FT kerosene exhibits properties representative of an FT-SPK blending component. Since the simulated kerosene does not explicitly include aromatic and cycloalkane components, the FT-SPK specification represents the most relevant primary benchmark. For comparison, the specification range for SPK/A is also considered. This comparison provides additional context regarding the potential influence of an appropriate synthetic aromatic fraction on the properties of synthetic kerosene. However, aromatic formation or addition is not explicitly represented in the present study. The simulated kerosene is not interpreted as demonstrating Annex A4 compliance. The reference values for critical properties, listed in Table 4, are taken from [5,27,28], which include critical properties such as density, flash point, and aromatic content, all of which are strongly dependent on the hydrocarbon composition of the fuel. Some specifications apply to both the FT-SPK and the SPK/A, while others are pathway-specific or feature differing limits. The final blending of the synthetic component with conventional Jet A/A-1 to produce the finished aviation fuel is outside the scope of the present study, which assesses the kerosene at the synthetic blending-component level.

2.7. Integration of Python-based kinetic model with process simulation

As described in Sections 2.3 and 2.4, the kinetic models for FT and HC are implemented in Python and integrated with Aspen Plus®. Fig. 2 illustrates the overall integration workflow between Aspen Plus® and Python-based kinetic model.

The workflow begins with reading required process parameters (T_{FT} , P_{FT} , X_i , X_{CO} , overall conversion) from the simulation using DLR in-house tool, PyTEEA [29]. Further, these parameters are passed to the FT kinetic model, where fractional conversion of CO ($X_{CO,i}$ fractional conversion) into the individual hydrocarbon components is calculated. The resulting conversion values are then written back into the simulation and the simulation file is executed. A detailed description of the FT kinetic model is described in the subsequent Section 2.7.1. Following this, the required process parameters for the HC kinetic model (n_i , T_{HC} , P_{HC} , $WHSV$) are extracted from the updated FT simulation file. These inputs are used to evaluate the reaction rates of individual component and subsequently, the corresponding product yields are written back into the simulation. Afterwards, the simulation file is executed again. The HC kinetic model is discussed in detail in the corresponding Section 2.7.2. As shown in Fig. 1, the HC recycle stream is treated iteratively by splitting it into two streams, as shown in Fig. 1:

Table 4
ASTM D7566 specification limit values [5,27,28].

Specification requirements	Unit	FT synthetic kerosene (FT-SPK) Annex A1		Synthetic kerosene with aromatics (SPK/A) Annex A4	
		Min	Max	Min	Max
Distillation temperature, 10 % recovered	°C	—	205	—	205
Final boiling point	°C	—	300	—	300
$T_{90}-T_{10}$	°C	22	—	22	—
Flash point	°C	38	—	38	—
Density at 15 °C	kg m ^{−3}	730	770	755	800
Viscosity at −20 °C	mm ² s ^{−1}	—	—	—	—
Viscosity at −40 °C	mm ² s ^{−1}	—	—	—	—
Aromatics	wt. %	—	0.5	—	20

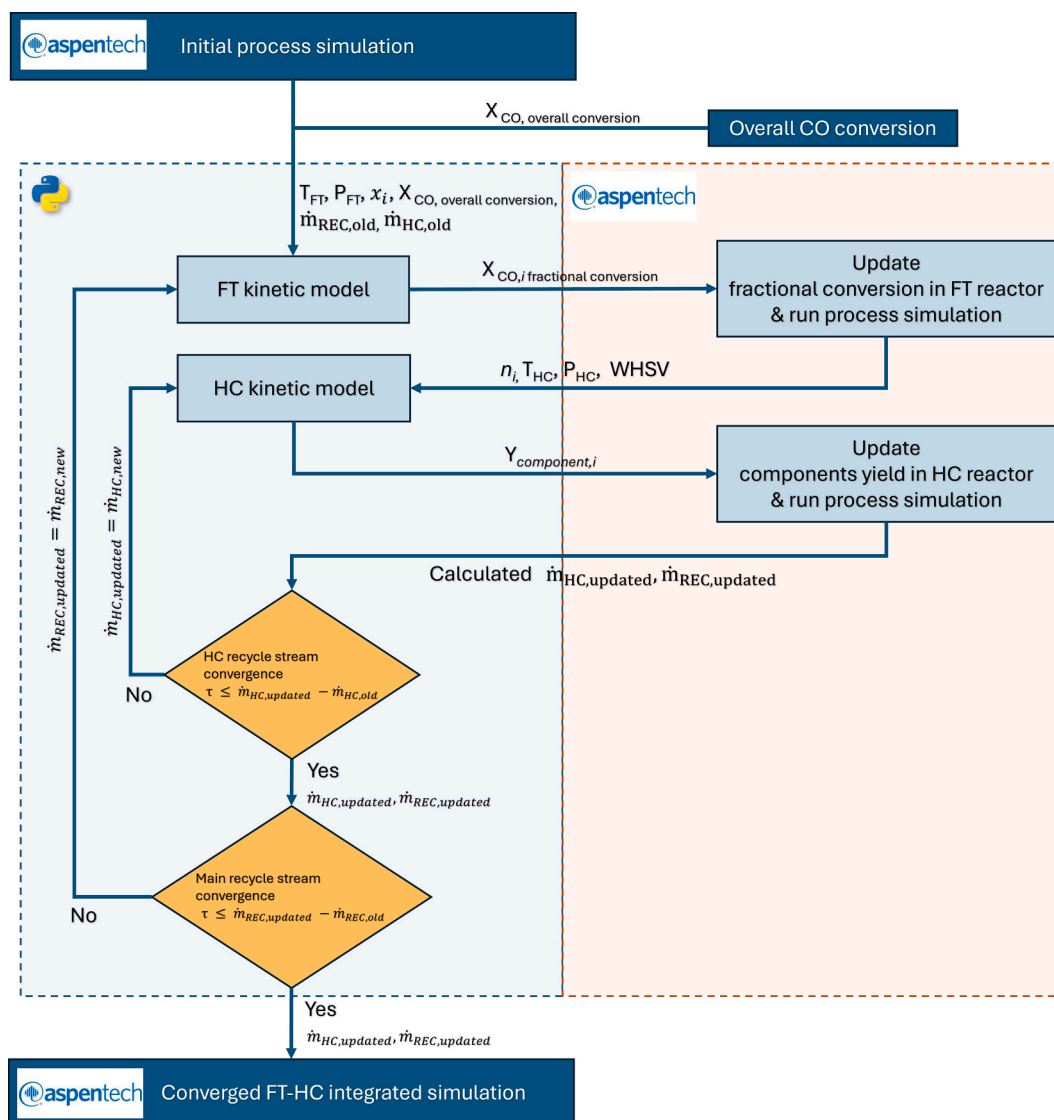


Fig. 2. Integration workflow between Aspen Plus® and Python-based kinetic model.

- The inlet stream to the HC reactor, representing the initial mass flow $\dot{m}_{HC,old}$.
- The outlet stream from the HC reactor, obtained after writing the product yields back into the HC block, representing the updated mass flow $\dot{m}_{HC,updated}$.

After executing simulation run, the difference in total mass flow and individual component mass flow between these two streams are checked against a predefined convergence tolerance. If the calculated difference exceeds the specified tolerance, the updated HC outlet mass flows $\dot{m}_{HC,updated}$ from the current iteration are reused as the recycle input stream $\dot{m}_{HC,new}$ for the subsequent iteration. This procedure is repeated until convergence is achieved. A similar iterative strategy is applied to the main recycle stream returning to the RWGS-FT synthesis loop, which is also split into two streams:

- The inlet recycle stream to the synthesis loop, representing the initial mass flow $\dot{m}_{REC,old}$.
- The resulting recycle stream from the synthesis loop, obtained after successful convergence of the HC reactor, representing the updated mass flow $\dot{m}_{REC,updated}$.

Once convergence of the HC recycle stream is achieved, the differences in total and individual component mass flow of these main recycle streams are also checked against the defined tolerance. If the convergence criterion is not satisfied, the updated FT outlet mass flows $\dot{m}_{REC,updated}$ obtained from the current iteration are reused as the recycle input stream $\dot{m}_{REC,new}$ for the subsequent FT kinetic model iteration. The FT-HC calculations are repeated iteratively until overall convergence of both recycle loops is obtained.

2.7.1. FT kinetic model

Due to inherent complexity of FT reaction kinetics, which involves multiple chain-growth reactions, and the limited flexibility of the Aspen Plus® reaction masks, the FT kinetics are implemented externally using a Python-based kinetic model. This approach allows greater flexibility in defining complex reaction rate expressions and allowed improved model customization compared to built-in Aspen Plus® models. In previous work [7], the kinetic model was implemented using Fortran user kinetic subroutine. In this study, the proposed kinetic model from [8] is implemented in Python. The implemented kinetic model is validated against literature data from [8], with details of the validation can be found in [7] as well as in SI chapter A3.1. The required process parameters for the kinetic equations comprise reaction

temperature, reaction pressure and component molar fractions. These inputs are extracted from the inlet stream and operating condition of the FT reactor. Based on these inputs, the kinetic model evaluates the reaction rates of individual components as per eq. 1–11. The combined reaction rates are then used to determine the overall CO consumption rate, which forms the basis for estimating the fractional conversion of CO. Using given target conversion of 55 % [7,9], the corresponding catalyst requirement is calculated, and the fractional CO conversion associated with individual reactions is evaluated and written back to simulation.

2.7.2. HC kinetic model

The HC kinetic model is developed using a LHHW framework integrated with vapor–liquid equilibrium (VLE), following the methodology proposed in Gambaro et al. [13]. Among the kinetic models presented by Gambaro et al. [13], the model M2 is adopted in this study, due to its demonstrated ability to accurately predict product distributions, capture the influence of operating condition on kinetic behavior, employ improved kinetic and thermodynamic parameters, and explicitly integrate VLE effects into the reaction kinetics. The HC kinetic model is based on the following assumptions adopted from [13]:

- n-paraffins undergoes isomerization to form iso-paraffins, which collectively represent all the possible isomers regardless of number, position, or chain length.
- Iso-butane is formed exclusively through cracking of heavier compounds and not via isomerization of n-butane.
- Iso-C₅ does not undergo cracking reactions.
- Iso-C_n, with $n > 5$ are subject to cracking.
- Iso-C₆, cracks to produce C₁–C₅ hydrocarbons.
- Iso-C₇, cracks to yield equimolar amounts of C₃ and iso-C₄.
- Cracking of iso-C_n ($n \geq 8$), follows a bond-breaking function.
- A uniform bond breaking probability (P) is assumed for C–C bonds between C₄ and C_{n-4}.
- A reduced bond-breaking probability (P/2) is applied to C₃ and C_{n-3}.
- The cracking probability for C–C bonds including C₁, C₂, C_{n-2}, C_{n-1}, C_n are assumed as zero.

The HC reactor is modelled as a plug flow reactor in Python, and discretized along the residence time (τ) coordinate. The reaction rates, specified in eq. 12–26, are calculated sequentially in each discretized reactor element until the total residence time is reached. The required process parameters to compute reaction rates including component molar and mass flow rates, temperature and pressure, are extracted from simulation, where the HC reactor is represented as a yield reactor. Total residence time is approximated as the inverse of WHSV, assuming constant catalyst density. Based on the initial molar compositions, VLE calculations are performed to determine component fugacities. Then at each discretized residence time step, the reaction rates are computed and used to calculate the changes in the molar flow rates of individual components. These changes are added to the inlet molar flows to obtain updated component compositions at the reactor outlet of that element. These updated molar compositions serve as a new input for the subsequent iteration. This iterative coupling of reaction rate computation and VLE ensures thermodynamic consistency throughout the reactor. The procedure is repeated until the cumulative residence time satisfies the termination criterion as shown in Fig. 3. Upon completion of the residence time loop, the final mass yields of all components are calculated and written into the HC reactor block in Aspen Plus®. The implemented kinetic model is validated against literature data from [13], with results provided in SI chapter A3.2.

3. Technical assessment methodology

For technical assessment, four efficiencies, kerosene yield and kerosene carbon efficiency are defined to compare the different case

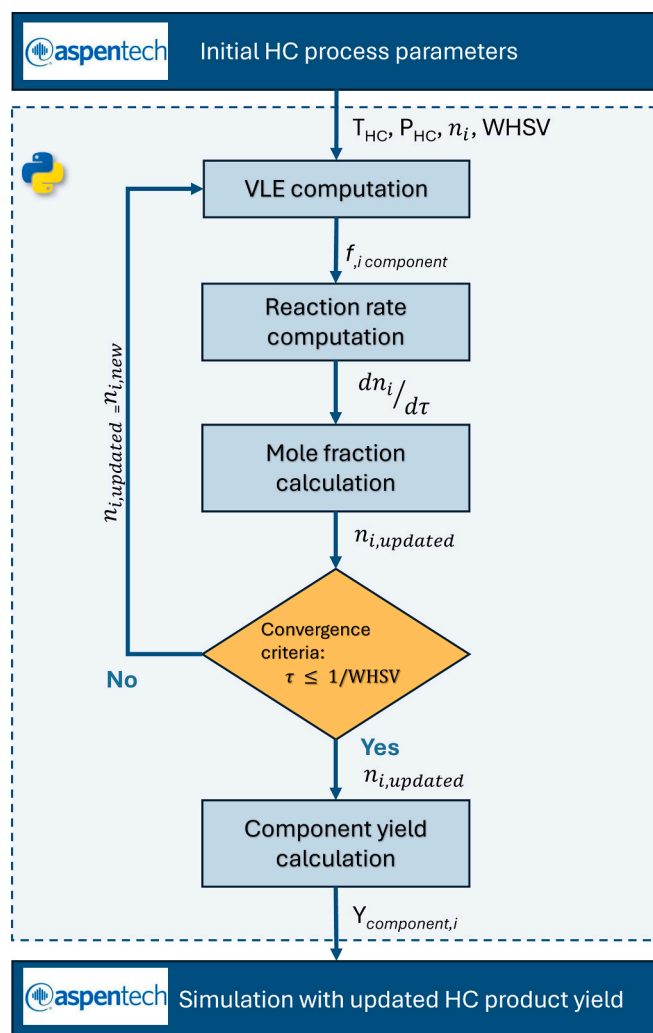


Fig. 3. Workflow of Python-based HC kinetic model and integration with Aspen Plus®.

studies. The Power-to-kerosene efficiency η_{ptk} , given by Eq. (31), relates the lower heating value ($LHV_{kerosene}$) of the produced fuel to the total electrical power input to the plant [30,31]. Similarly, the Power-to-liquid efficiency η_{ptl} , given by Eq. (32), relates the lower heating value ($LHV_{totalproduct}$) of the total produced fuel to the total electrical power input to the plant [30,31].

$$\eta_{ptk} = \frac{\dot{m}_{kerosene} \cdot LHV_{kerosene}}{P_{el}} \quad (31)$$

$$\eta_{ptl} = \frac{\dot{m}_{totalproduct} \cdot LHV_{totalproduct}}{P_{el}} \quad (32)$$

Here, $\dot{m}_{kerosene}$, $\dot{m}_{totalproduct}$ denote the mass flow rates of the produced kerosene and total products, respectively, while P_{el} is the total electrical power supplied. The definition of the kerosene fraction is based on the fuel properties as listed in the Table 4, in particular flash point, viscosity and boiling point cut.

The Hydrogen-to-kerosene efficiency (η_{H2tk}) describes the efficiency with which the chemical energy of hydrogen is converted into the chemical energy of kerosene. It is a more appropriate indicator for assessing conversion improvements, as it excludes the electrolyser losses, which are defined by the electrolyser efficiency. It is defined as the ratio of the $LHV_{kerosene}$ of the produced kerosene to the LHV_{H_2} of the H_2 input utilized in the synthesis [30,31]. Likewise, the conversion of hydrogen chemical energy into the total liquid products energy is

described by the Hydrogen-to-liquid efficiency (η_{HtL}).

$$\eta_{HtL} = \frac{\dot{m}_{kerosene} \bullet LHV_{kerosene}}{\dot{m}_{H_2} \bullet LHV_{H_2}} \quad (33)$$

$$\eta_{HtL} = \frac{\dot{m}_{totalproduct} \bullet LHV_{totalproduct}}{\dot{m}_{H_2} \bullet LHV_{H_2}} \quad (34)$$

Here, $\dot{m}_{H_2}$ is the mass flow rate of the H_2 feed.

The kerosene yield ($y_{kerosene}$) is defined as the ratio of the mass flow of the kerosene in the product stream ($\dot{m}_{kerosene}$) to the mass flow of the total liquid product stream ($\dot{m}_{liquidproduct}$), as described in Eq. (35).

$$y_{kerosene} = \frac{\dot{m}_{kerosene}}{\dot{m}_{liquidproduct}} \quad (35)$$

The kerosene carbon efficiency (η_C) is defined as the ratio of the carbon mass flow in the kerosene stream ($\dot{m}_{C,kerosene}$) to the carbon mass flow in the CO_2 feed ($\dot{m}_{C,CO_2feed}$), as described in Eq. (36).

$$\eta_C = \frac{\dot{m}_{C,kerosene}}{\dot{m}_{C,CO_2feed}} \quad (36)$$

4. Economic assessment methodology

The methodology used to estimate the equipment cost (EC_i), fixed capital investment (FCI), annual capital cost (ACC), and operating cost follows the approach proposed in [31–33]. The cost estimation is expected to have an accuracy of $\pm 30\%$ for well-known chemical processes [33], according to class three and four of classification system for association for Advancement of Cost Engineering [34]. General plant assumptions are shown in Table 5. Norway is considered as the plant location, due to its electricity mix, which is almost entirely based on renewable sources [35]. Norway is also at the forefront of SAF adoption in Europe, driven with its early implementation of the ReFuelEU Aviation regulations [36]. In addition, Norway has significant potential for the supply of biogenic CO_2 , supported by the active deployment of bioenergy with carbon capture and storage (BioCCS) in multiple waste-to-energy plants and the integration of biomass use with CCS in industrial plants [37].

The main outcome of economic assessment is the net production costs (NPC), defined in Eq. (37).

$$NPC \left[\frac{\text{€}}{MWh_{LHV}} \right] = \frac{ACC + \sum OPEX_{dir} + \sum OPEX_{ind} + t_{labor} \bullet c_{labor}}{\dot{m}_{kerosene} \bullet LHV_{kerosene}} \quad (37)$$

Where, ACC denotes the annual capital cost, $OPEX_{dir}$ and $OPEX_{ind}$ represents the direct and indirect operational expenditure, respectively. Furthermore, t_{labor} is the annual labor requirement and c_{labor} denotes the specific labor cost, as reported in Table 6.

Direct OPEX comprise expenditures associated with feedstocks, utilities and energy consumption, as summarized in Table 6, whereas

Table 5
General assumptions for the FT-plant.

General plan assumptions		
Location	Norway	Country-specific electricity price and labor cost applied
Plant capacity	1.8 t h ⁻¹ H ₂	Based on a 100 MW _{el} PEM electrolyser operating at overall efficiency of 60 %
Full load hours	8,000 h a ⁻¹	Accounts for scheduled and unscheduled maintenance downtime [31]
Plant operating lifetime	20 years	Taken from [31,38,39]
Interest rate	7 %	Taken from [40]
Base year	2024	Cost base year for evaluation, using CEPCI-adjusted values
Site	Brownfield	Existing chemical plant site with assumed access to utilities and infrastructure

Table 6
Specific cost for raw materials, utilities and by-products.

	Price	Unit	Remarks	Ref
<i>Raw materials and utilities</i>				
Electricity	97.5	€ ₂₀₂₄ MWh ⁻¹	considered for Norway	[41]
Labor cost	60.1	€ ₂₀₁₆ h ⁻¹	considered for Norway	[42]
CO ₂ cost	80	€ ₂₀₂₄ t ⁻¹	Derived from a land-based biomass incineration plant	[31]
<i>Byproducts</i>				
E-gasoline	2.3	€ ₂₀₂₅ l ⁻¹	Average price	[43]
E-diesel	2.7	€ ₂₀₂₅ l ⁻¹	Average price	[43]

indirect OPEX account for additional operating expenses, including maintenance, labor, insurances, administration, and taxes [32]. Labor requirements are estimated using the rule of thumb approach proposed by Peter et al. [31,32], assuming large scale equipment, highly automated or fluid processing systems. The economic surcharge factors used for Indirect OPEX estimation are provided in the SI Table A.7.

ACC is determined from the Fixed capital investment cost (FCI), Interest rate (IR), plant depreciation time (y) and working capital, according to Eq. (38).

$$ACC = FCI \bullet IR \bullet \left(\frac{(1 + IR)^y}{(1 + IR)^y - 1} + \frac{1}{1 - \text{workingcapital}} - 1 \right) \quad (38)$$

FCI is estimated using the purchase equipment cost EC_i and corresponding empirical factors $F_{eco,i,j}$ as given in Eq. (39).

$$FCI = \sum EC_i \bullet \left(1 + \sum_{j=1}^{10} F_{eco,i,j} \right) \left(1 + \sum_{j=11}^{12} F_{eco,i,j} \right) \quad (39)$$

EC_i is calculated from the specific equipment cost correlations as a function of the characteristic sizing parameters $S_{i,k}$, such as pressure, temperature, and throughput.

$$EC_i = f_i(S_{i,1}, \dots, S_{i,k}) \bullet \left(\frac{CEPCI}{CEPCI_{ref(i)}} \right) \bullet F_{material,i} \bullet F_{pressure,i} \text{ for } i, k \in \mathbb{N} \quad (40)$$

The cost correlations are adjusted to the economic conditions of the evaluation year using the chemical engineering plant cost index (CEPCI), while $F_{material,i}$ and $F_{pressure,i}$ account for material selection and operating pressure, respectively. The cost of standard equipment, such as flash drums, pumps, compressors, heat exchangers are estimated based on [32]. The cost sizing parameters and fixed capital investment costs of the equipment are summarized in the SI Table A.1-A.3.

Based on the calculated FCI, the total capital investment (TCI) is calculated using Eq. (41), assuming a working capital of 15 % [33]. TCI represents the total capital required for the chemical plant, including both FCI and working capital.

$$TCI = \frac{FCI}{1 - \text{workingcapital}} \quad (41)$$

5. Results and discussion

This section presents the results of technical and economical assessment, with detailed focus on the influence of FT and HC operating conditions on kerosene yield, process efficiency, carbon distribution, SAF specification compliance, and kerosene production cost.

5.1. Technical assessment

The technical assessment comprises the parameter study of FT and HC operating conditions, the selection of the representative cases for further assessment, process efficiencies, carbon flow analysis, and verification of the kerosene specifications.

5.1.1. Parameter study

As described in the Section 2.4, the selected HC operating parameters were systematically varied as listed in Table 3. Fig. 4 illustrates the influence of these HC operating parameters on the kerosene yield. To isolate the effect of HC, the operating condition of the RWGS step was kept constant throughout the parameter study. Fig. 4 shows the HC parametric study for two FT operating conditions: a) 220 °C, 25 bar and H₂/CO molar ratio of 1.6 and b) 230 °C, 25 bar and H₂/CO molar ratio of 2.

As shown in Fig. 4a, higher kerosene yield of 87.6 % is achieved at complete wax conversion under HC operating conditions of 35 bar, 378 °C and WHSV of 1 h⁻¹ (straight lines). At this temperature and WHSV, increasing the pressure to 45 bar and 55 bar results in a slight decrease in kerosene yield to 87.3 % and 86.8 %, respectively. This behavior reflects the well-known pressure effect on hydrocracking severity, where higher pressure suppresses C–C bond cleavage, resulting in a modest reduction in cracking severity [27]. At lower temperatures (373 °C and 368 °C) and constant WHSV of 1 h⁻¹, the kerosene yield further decreases with increasing HC operating pressure (45 bar and 55 bar), confirming that cracking severity is enhanced at higher temperatures and lower pressures. In particular, at 368 °C, a significant drop in kerosene yield is observed compared to 378 °C and 373 °C. This reduction is primarily attributed to incomplete wax conversion, due to insufficient cracking severity, especially at elevated pressure of 55 bar. As a consequence, the HC recycle stream increases, leading to a higher fraction of unconverted heavy hydrocarbons being recycled back from the distillation column (Column-1) to the HC reactor. This recycle stream enriches the feed with heavier hydrocarbons (C₁₇₊) and reduces the effective per-pass conversion, thereby lowering the overall kerosene yield. A similar trend can be seen at a higher WHSV 1.5 h⁻¹ (dotted lines). However, the maximum achievable kerosene yield is significantly lower (74.5 %) compared to the case at 1 h⁻¹. This indicates that higher WHSV limits residence time and wax conversion, thereby lowering the kerosene yield.

Fig. 4b presents the HC parametric study under severe FT operating condition (230 °C, 25 bar, 2 H₂/CO molar ratio). The observed trend aligns with that from the milder FT condition (220 °C, 25 bar, 1.6 H₂/CO molar ratio), where kerosene yield increases with increasing HC temperature, decreasing pressure and decreasing WHSV. However, it is interesting to note that the maximum kerosene yield declines from 87.6 % to 85.9 %, under the severe FT case. This modest decline is attributable to the intrinsic FT kinetics at the more severe synthesis

conditions. The elevated temperature accelerates 1-olefin desorption from growing surface species, while the higher H₂/CO ratio lowers CO partial pressure and raises H₂ partial pressure, decreasing adsorbed CO coverage for chain propagation. Both effects lower the α value, a behavior that is well established for cobalt-based FT synthesis [44] and is also captured by the kinetic model used in this study. As a result, the asymptotic α value is 0.948 at the severe FT condition, compared with 0.966 at the milder FT condition, as mentioned in Table 7.

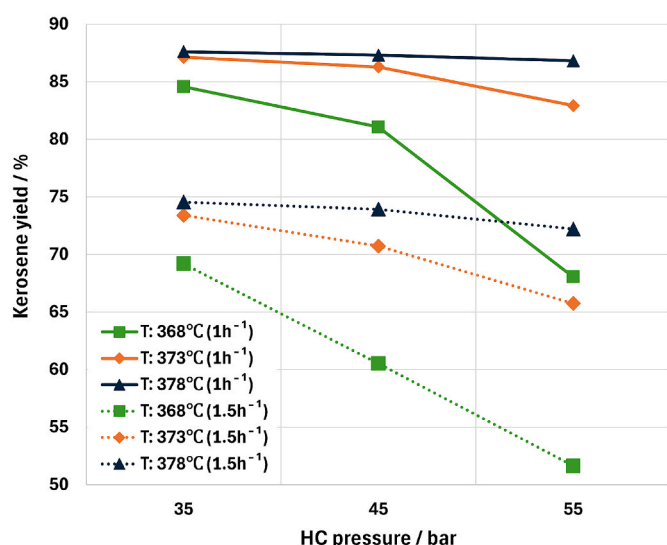
This decrease in α value is clearly reflected in the FT product distribution, shown in Fig. 5, which compares the paraffinic and olefinic fractions at the FT reactor outlet for both FT conditions. The lower α at severe FT conditions promotes earlier chain termination, shifting the paraffinic and olefinic distributions toward lighter hydrocarbons. Conversely, the mild condition sustains a higher α value, yielding heavier paraffins. This is evident from the crossover in the paraffinic distribution near C₁₉–C₂₀ (Fig. 5a), beyond which C₂₀–C₃₀ mass flow remains consistently higher for the milder condition. Furthermore, methane formation increases by approximately 108 % at the severe FT condition compared with the milder condition, consistent with methane being the terminal product of chain termination at low α . Consequently, the severe FT condition generates a larger main recycle stream flow relative to the mild FT condition, reducing the streamflow available for downstream upgrading. Hence, this limits the attainable kerosene yield to 85.9 %. Moreover, under the more severe cracking condition in the HC (378 °C, 35 bar, 1 h⁻¹) coupled with the severe FT condition, the cracking intensity becomes sufficient to break a substantial portion of kerosene-range hydrocarbons, increasing the gasoline fraction and further limiting the kerosene yield to 85.7 %. Similar parametric trends for the remaining FT operating conditions are provided in SI figure A.2 and A.3.

Fig. 6 presents the resulted kerosene yield obtained from HC parametric study under four FT operating conditions as indicated at the bottom of the Fig. 6. It can be seen, that kerosene yield of more than 80 % is achievable with FT process optimization in a rather broad spectrum

Table 7
Asymptotic chain growth probability for the two FT conditions.

FT condition	Asymptotic α values
220 °C, 25 bar, 1.6 H ₂ /CO molar ratio	0.966
230 °C, 25 bar, 2 H ₂ /CO molar ratio	0.948

a) FT condition: 220 °C, 25 bar and 1.6 H₂/CO molar ratio



b) FT condition: 230 °C, 25 bar and 2 H₂/CO molar ratio

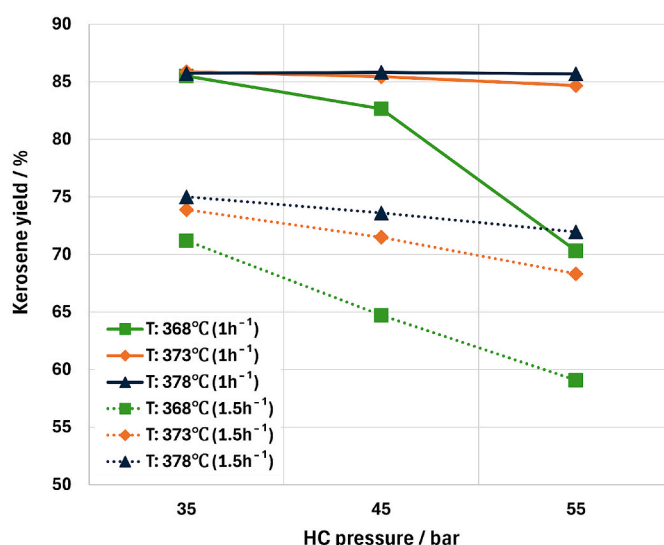


Fig. 4. HC parameter study (pressure 35–55 bar, temperature 368 – 378 °C, WHSV of 1–1.5 h⁻¹) at different FT operating condition.

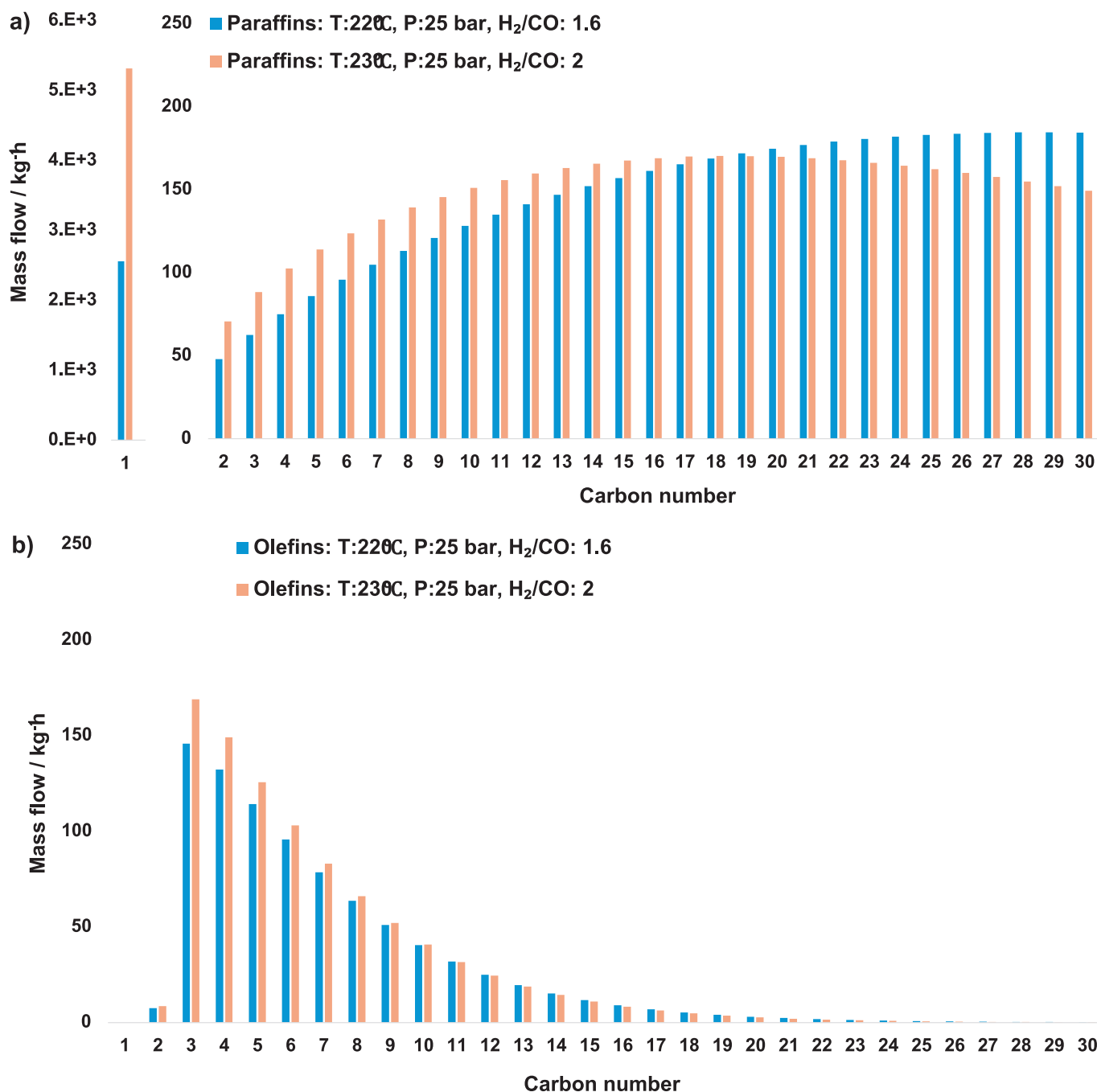


Fig. 5. FT reactor outlet hydrocarbon distribution for two FT conditions (220°C, 25 bar, 1.6 H₂/CO molar ratio and 230°C, 25 bar, 2 H₂/CO molar ratio): a) Paraffin distribution and, b) Olefin distribution.

of process parameters. The results highlight a strong dependence of kerosene yield on both upstream FT synthesis and downstream HC operating parameters. Across all FT cases shown in Fig. 6, the kerosene yield increases with increasing HC temperature, decreasing pressure and decreasing WHSV, consistent with the trends discussed previously. The highest kerosene yield of 87.6 % is achieved at the FT condition of 220 °C, 25 bar and H₂/CO molar ratio of 1.6, under the most severe HC conditions (378 °C, 35 bar, 1 h⁻¹). In contrast, under less severe HC conditions (368 °C, 55 bar, 1.5 h⁻¹), the kerosene yield decreases significantly, reaching a minimum of 51.6 % for the same FT condition. Comparison across FT operating conditions shows that milder FT conditions favor higher downstream kerosene yields. This is attributed to a heavier FT product distribution with higher wax content, which

enhances the potential for kerosene production during hydrocracking. In contrast, less severe HC conditions shift the product spectrum toward lighter hydrocarbons, thereby limiting the maximum achievable kerosene yield.

5.1.2. Process efficiencies

For the further assessment, three cases were selected from the parameter study (see Fig. 6), as listed in Table 8.

- **Case 1 – Maximum kerosene yield:** corresponding to the highest kerosene yield in the parameter study. This represents the reference scenario for further evaluation.

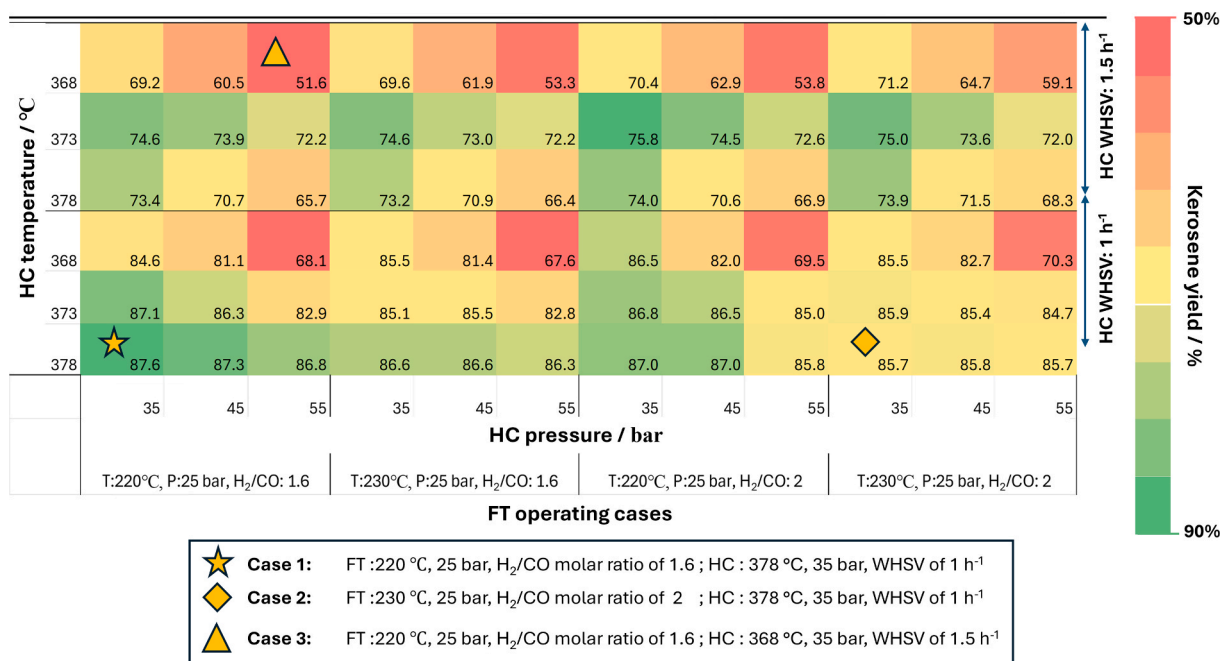


Fig. 6. Kerosene yield obtained from HC parametric study under four FT operating conditions.

Table 8

Selected process configuration cases for technical and economic assessment.

	Unit	Case 1 Maximum kerosene yield	Case 2 Higher gasoline co-production	Case 3 Higher diesel co-production
FT Temperature	°C	220	230	220
FT Pressure	bar	25	25	25
H ₂ /CO ratio	–	1.6	2	1.6
HC Temperature	°C	378	378	368
HC pressure	bar	35	35	55
HC WHSV	h ⁻¹	1	1	1.5
Main recycle flow	kg h ⁻¹	25,342	28,061	25,313
HC recycle flow	kg h ⁻¹	4,640	3,946	12,724

- **Case 2 – Higher gasoline co-production:** corresponding to a high-severity operation of the FT and HC, resulting in a relatively higher gasoline fraction compared to Case 1. This case is included to evaluate the potential benefit of e-gasoline price, thereby achieving lowest kerosene production cost among the selected cases.
- **Case 3 – Higher diesel co-production:** lowest kerosene yield case, characterized by a higher fraction of diesel-range hydrocarbons compared to Case 1. This case is included to assess the benefit of higher e-diesel market value on the kerosene production cost.

These three cases were selected from the full set of 72 operating points to span the range from the highest kerosene yield (Case 1) to the operating extremes that most influence kerosene production cost through by-product credits (Case 2 and Case 3). These cases also allow to evaluate the impact of the product distribution and byproduct formation on technical process efficiencies and the overall economic value of kerosene production. Table 8 summarizes the corresponding FT and HC operating conditions, along with the internal HC recycle stream flow and the main recycle stream flow.

Table 9 presents the corresponding process efficiencies. Case 1 achieves the highest η_{PtK} of 34.8 %, followed by Case 2 (33.3 %) and Case 3 (20.9 %). This trend is directly linked to the kerosene production rate, which decreases significantly from Case 1 to Case 3. In Case 3, a substantial portion of the carbon is retained in the diesel fraction rather than being converted into kerosene, leading to a lower η_{PtK} efficiency. A similar trend is observed for η_{H2tk} , where Case 1 shows the highest

Table 9

Product mass flows and process efficiencies.

	Unit	Case 1 Maximum kerosene yield	Case 2 Higher gasoline co-production	Case 3 Higher diesel co-production
Kerosene	kg h ⁻¹	3,569	3,457 (–3 %)	2,119 (–41 %)
Gasoline	kg h ⁻¹	341	406	249
Diesel	kg h ⁻¹	163	169	1,735
Total Product	kg h ⁻¹	4,073	4,032 (–1 %)	4,103 (+0.7 %)
η_{PtK}	%	34.8	33.3	20.9
η_{H2tk}	%	69.0	66.8	40.9
η_{PtL}	%	39.9	39.1	41.1
η_{H2tL}	%	79.2	78.4	80.4
η_{C}	%	86.9	84.5	51.4

efficiency with 69.0 %, while Case 2 decreases slightly (66.8 %) due to increased formation of gasoline-range hydrocarbons. In Case 3, the η_{H2tk} drops significantly to 40.9 %, primarily due to lower wax conversion, which reduces the effective utilization of hydrogen in producing kerosene-range hydrocarbons. This behavior is further reflected in the η_{C} . Case 1 achieves the highest kerosene carbon efficiency (86.9 %), followed by Case 2 (84.5 %) and Case 3 (51.4 %). In contrast, η_{PtL} and

η_{H2L} follow the opposite trend, with Case 3 highest (η_{PIL} 41.1 % and η_{H2L} 80.4 %), followed by Case 1 and Case 2. This inversion reflects the conversion of the carbon and hydrogen not converted to kerosene in Case 3 are retained in the diesel fraction, so the overall liquid efficiencies remain high.

5.1.3. Carbon flow analysis

Fig. 7 presents the carbon flow distribution across the process units for three selected cases. Sankey diagrams illustrate how carbon is transferred through each process unit and ultimately distributed among different hydrocarbon product groups. The component grouping represents various hydrocarbon classes across product ranges including light gases, naphtha, kerosene, diesel, and wax fractions. For all cases, the carbon input is maintained nearly constant to achieve the required H_2/CO molar ratio for the FT synthesis, as specified in Table 8. The CO_2 feed is introduced into the RWGS unit, along with recycle stream from the FT synthesis and product separation unit. While the CO_2 input remain similar across cases, the recycle stream to the RWGS varies significantly. This recycle stream is primarily composed of unconverted gases such as CO , CO_2 , CH_4 , and light gases. A notable difference is observed in Case 2, where a relatively larger recycle stream is going to the RWGS unit. This is attributed to the severe FT operating conditions (230 °C and 2 H_2/CO molar ratio), which promote the formation of methane and light gases, as depicted in Fig. 5. As a result, less carbon is converted into long chain hydrocarbons for downstream upgrading. The carbon flow also describes the differences in reactor sizing among the cases summarized in Table 10. Due to the severe FT condition in Case 2, the target CO conversion of 55 % is achieved with a smaller FT reactor volume of 71 m^3 compared with 126 m^3 in Cases 1 and 3. Consequently, the carbon flow of light hydrocarbons directed to the hydrotreating section is highest in Case 2 (approximately 33 %), compared to 27 % in Cases 1 and Case 3.

Significant differences are also observed in the hydrocracking section. While the carbon flow from the FT synthesis to the HC unit is similar for Cases 1 and 3, the HC operating conditions determine the extent of wax conversion. In Case 3, less severe hydrocracking condition results in incomplete wax conversion, generating a substantially larger internal HC recycle stream including diesel- and wax-range paraffinic and iso-paraffinic compounds. Consequently, the HC experiences highest throughput and requires the largest reactor sizing. In contrast, Cases 1 and 2 achieve complete wax conversion, and the corresponding HC recycle stream consists mainly of heavier iso-paraffinic hydrocarbons. This indicates more effective upgrading of heavy fractions and reduced internal recirculation. The carbon flow through the product separation unit is relatively similar across all cases. Light gases are separated and recycle back to the RWGS unit, maintaining overall carbon utilization within the system. However, the final carbon distribution to products differs significantly. Case 1 shows the highest carbon selectivity towards kerosene (86.9 %), followed by Case 2, while Case 3 exhibits a much lower kerosene fraction of 51 %, with a larger portion of carbon remaining in diesel fraction.

5.1.4. Product specifications

Table 11 presents the calculated fuel properties for the three representative cases alongside the specification limits for FT-SPK and SPK/A according to ASTM D7566 [15]. Overall, the kerosene stream from the simulated model satisfies the majority of the evaluated specification criteria, with density representing the principal deviation. The calculated 10 % recovery temperature is 153.5 °C for all three cases, while the final boiling points are 251.3, 251.5, and 251.4 °C for Cases 1–3, remaining well below the upper specification limit of 300 °C. The T_{90-T10} values are also within the relevant specifications, indicating an appropriate distillation profile for the simulated kerosene. As described in Section 2.5, the flash point of 38 °C is imposed as a design target in the distillation column by varying the distillate-to-feed ratio, selected to maximize the kerosene yield while satisfying the minimum flash point requirement. The resulting separation performance, including

distillation stages, reboiler duty and condenser duty, is reported for each case in the Supplementary Table A.4–A.6. Further tuning of the product separation was not considered in the present study. The calculated density at 15 °C is 723, 724 and 727 $kg\ m^{-3}$ for Cases 1–3, compared with the FT-SPK range of 730–770 $kg\ m^{-3}$. Thus, the calculated density is approximately 3–7 $kg\ m^{-3}$ below the FT-SPK minimum. Since the final boiling point remains well below the 300 °C limit, the distillation cut could be shifted toward heavier paraffins, which may provide additional flexibility to raise the density toward the FT-SPK range. However, such an adjustment would also influence the flash point, product recovery, and energy requirements, and would therefore require further optimization of the separation conditions, which is beyond the scope of the present study. The density difference is more pronounced relative to the higher SPK/A range, for which an aromatic fraction is required. This larger difference reflects the absence of aromatic and cycloalkane components in the present model, as these hydrocarbon classes increase the density of synthetic kerosene. Their incorporation was not included in the present model, as it is outside the scope of this study.

5.2. Economic assessment

Fig. 8 illustrates the NPC of kerosene for the three selected cases, including CAPEX, OPEX and credits from by-product revenues. Among the evaluated cases, Case 2 exhibits the lowest NPC at 6.2 $\text{€}_{2024}\ kg_{kerosene}^{-1}$, followed by Case 1 with 7.0 $\text{€}_{2024}\ kg_{kerosene}^{-1}$, while Case 3 shows the highest NPC of 9.1 $\text{€}_{2024}\ kg_{kerosene}^{-1}$. Electricity represents the dominant cost contributor in all cases, accounting for approximately 45 % of the total cost in Case 1, 53 % in Case 2, and 58 % in Case 3. The increasing share of electricity cost across cases highlights the strong dependence of the cost on the kerosene yield and the process efficiencies. Consequently, the electrolyser constitutes the largest CAPEX contributor, with cost contributions of 0.9, 1.0 and 1.6 $\text{€}_{2024}\ kg_{kerosene}^{-1}$ for Cases 1, 2, and 3, respectively. The process configuration includes four reactors including RWGS, FT, HT and HC. Among these units, the FT and HC reactors represents the most significant capital contributors, accounting for approximately 9 %, 9 %, and 15 % of the NPC for Cases 1, 2, and 3, respectively, as shown in Table 10. The HC cost in Case 3 is approximately 9 % which is significantly higher than the other cases due to large HC internal recycle stream. The incomplete wax conversion nearly doubles the HC reactor throughput, increasing the reactor size by 96 % compared to Case 1. This behavior is already discussed in Section 5.1 and summarized in Table 8. Similarly, the FT reactor cost is higher in Case 1 compared to Case 2, due to the larger synthesis loop recycle stream, which results in increased reactor capacity.

In addition to CAPEX, indirect OPEX which is calculated based on FCI, also contributes significantly to the overall cost. Its accounting for approximately 32 % (Case 1), 35 % (Case 2) and 39 % (Case 3), reflecting the larger equipment sizes and overall plant investment required under these operating conditions. Another important factor affecting the NPC is the revenue from the by-products, primarily e-gasoline and e-diesel. While the gross production cost of kerosene (excluding by-product credits) is 8.2 $\text{€}_{2024}\ kg_{kerosene}^{-1}$ lower in the maximum kerosene yield case (Case 1) in comparison to Case 2 and Case 3. However, the total revenue generated from by-products is significantly higher in Case 2 (2.1 $\text{€}_{2024}\ kg_{kerosene}^{-1}$) and Case 3 (4.6 $\text{€}_{2024}\ kg_{kerosene}^{-1}$). This is due to the larger quantities of gasoline and diesel produced in these cases, which have substantial market value. As a result, higher by-product revenue in Case 2 offsets the gross production cost, ultimately leading to the lowest overall NPC among the evaluated cases.

5.3. Sensitivity analysis

The sensitivity analysis was performed to assess the influence of key

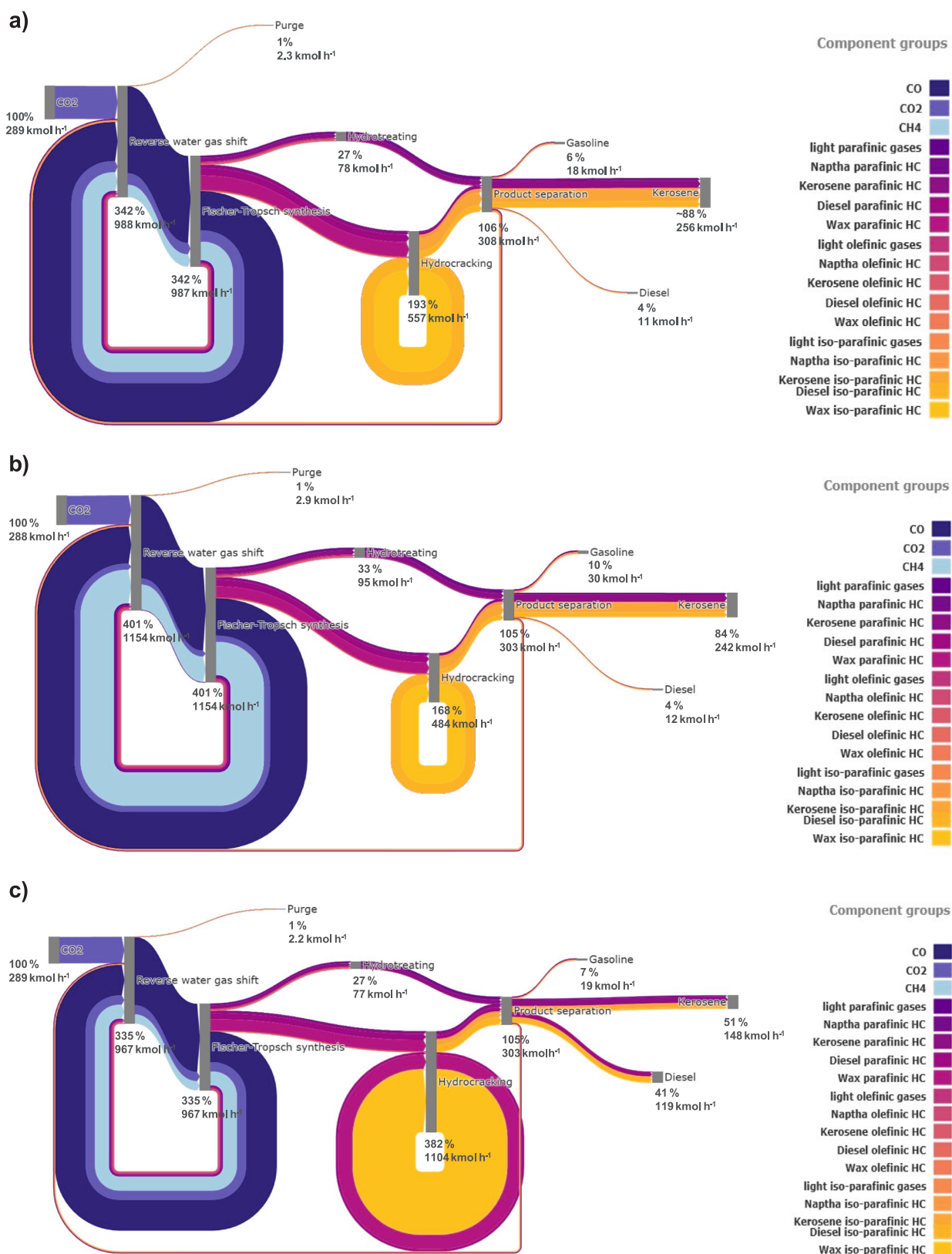


Fig. 7. Carbon flow distribution across the process units for three selected cases, a) Case 1: Maximum kerosene yield b) Case 2: Higher gasoline co-production and c) Case 3: Higher diesel co-production.

Table 10
Equipment sizing and basis for cost estimation.

Reactors	Sizing parameter	Unit	Case 1 Maximum kerosene yield	Case 2 Higher gasoline co-production	Case 3 Higher diesel co-production
Fischer-Tropsch	Volume	m ³	126	71 (−44 %)	126 (+0 %)
Hydrotreater	Throughput	kg h ^{−1}	1,126	1,366 (+21 %)	1,126 (+0 %)
Hydrocracker	Throughput	kg h ^{−1}	8,889	7,450 (−16 %)	17,427 (+96 %)
Reverse water gas shift	Throughput	kg h ^{−1}	39,856	42,528 (+7 %)	39,848 (−0.02 %)

raw materials costs including electricity price, CO₂ price and by-product prices (e-gasoline and e-diesel) on the NPC of kerosene, as depicted in Fig. 9. Among the raw materials, electricity price exhibits the most significant impact, reflecting its dominant role in H₂ production within the PtL processes. Case 2 remains economically favorable compared to

Case 1. However, at electricity prices above approximately 260 € MWh^{−1}, its NPC exceeds that of Case 1. In contrast, Case 3 exhibits the highest sensitivity to electricity price due to its lower η_{PtL} . As a result, Case 3 is generally less attractive than Case 1, but a break-even point is reached at an electricity price of approximately 10 € MWh^{−1}, below which Case 3 economically favorable.

In contrast, the effect of CO₂ price is comparatively small and nearly linear for all cases, indicating that the overall NPC is considerably less sensitive to CO₂ price than to electricity price. The influence of by-product prices is more case-dependent. The e-gasoline price strongly affects Case 2, where gasoline production is relatively higher than other cases. A break-even point is observed at an e-gasoline price of approximately 0.2 € l^{−1}, below which the economic advantage of Case 2 relative to Case 1 is diminished. Similarly, e-diesel price has minimal impact on the Case 1 and Case 2 but substantially influences the economics of Case 3. At e-diesel prices above approximately 4.3 € l^{−1}, a break-even point is reached, resulting in a lower NPC for Case 3 than for Cases 1. These results demonstrate that, in addition to raw material prices, the market value of by-products can significantly influence kerosene production costs.

Table 11
Product specifications.

	Unit	Case 1 Maximum kerosene yield	Case 2 Higher gasoline co-production	Case 3 Higher diesel co-production	FT-SPK		SPK/A	
Specification requirements					Min	Max	Min	Max
Distillation temperature, 10 % recovered	°C	153.5	153.5	153.5	—	205	—	205
Final boiling point	°C	251.3	251.5	251.4	—	300	—	300
T ₉₀ -T ₁₀	°C	85.6	85.0	83.3	22	—	22	—
Flash point	°C	38	38	38	38	—	38	—
Density at 15 °C	kg m ^{−3}	723	724	727	730	770	755	800
Viscosity at −20 °C	mm ² s ^{−1}	4.4	4.4	4.3	—	—	—	—
Viscosity at −40 °C	mm ² s ^{−1}	6.9	6.8	6.7	—	—	—	—
Aromatics	wt.%	—	—	—	—	0.5	—	20

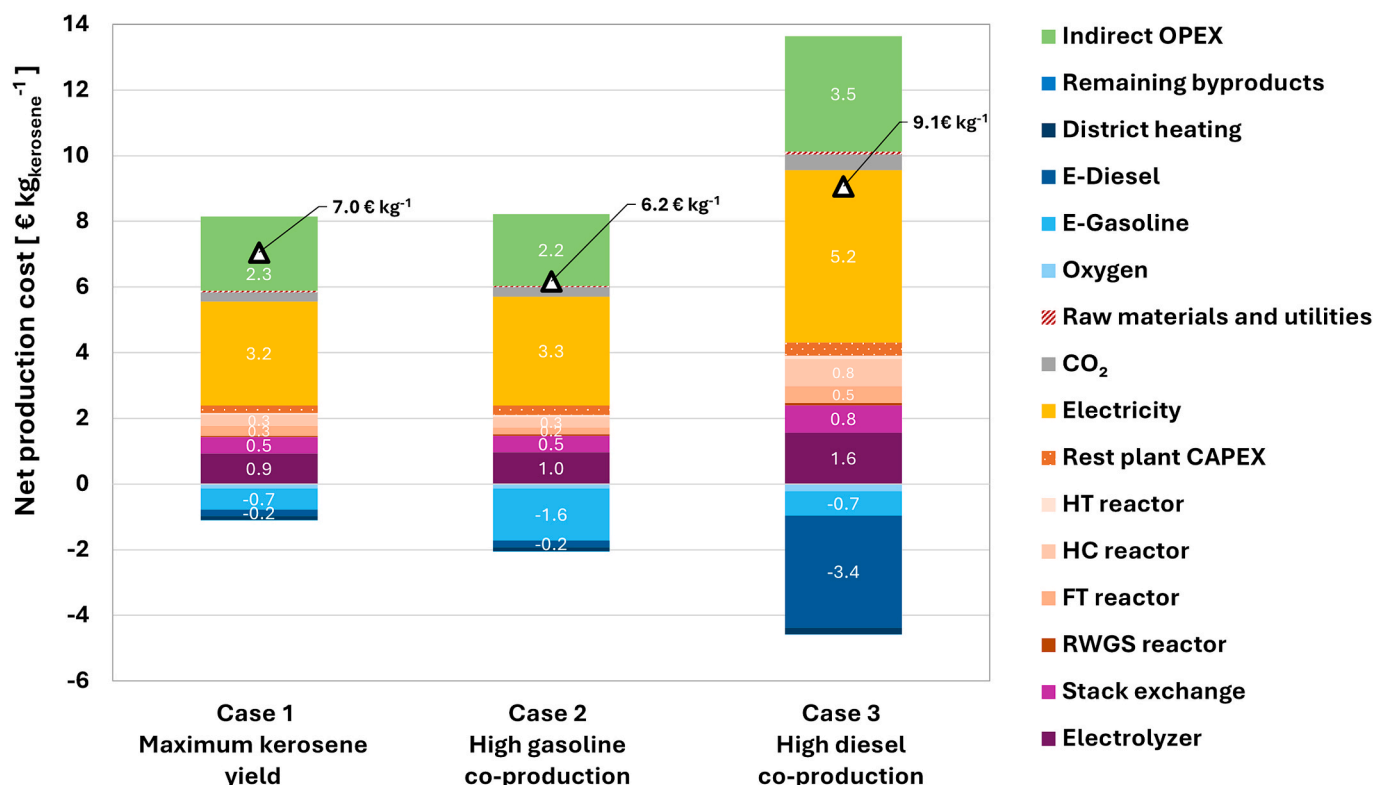


Fig. 8. Net production cost of FT-kerosene process.

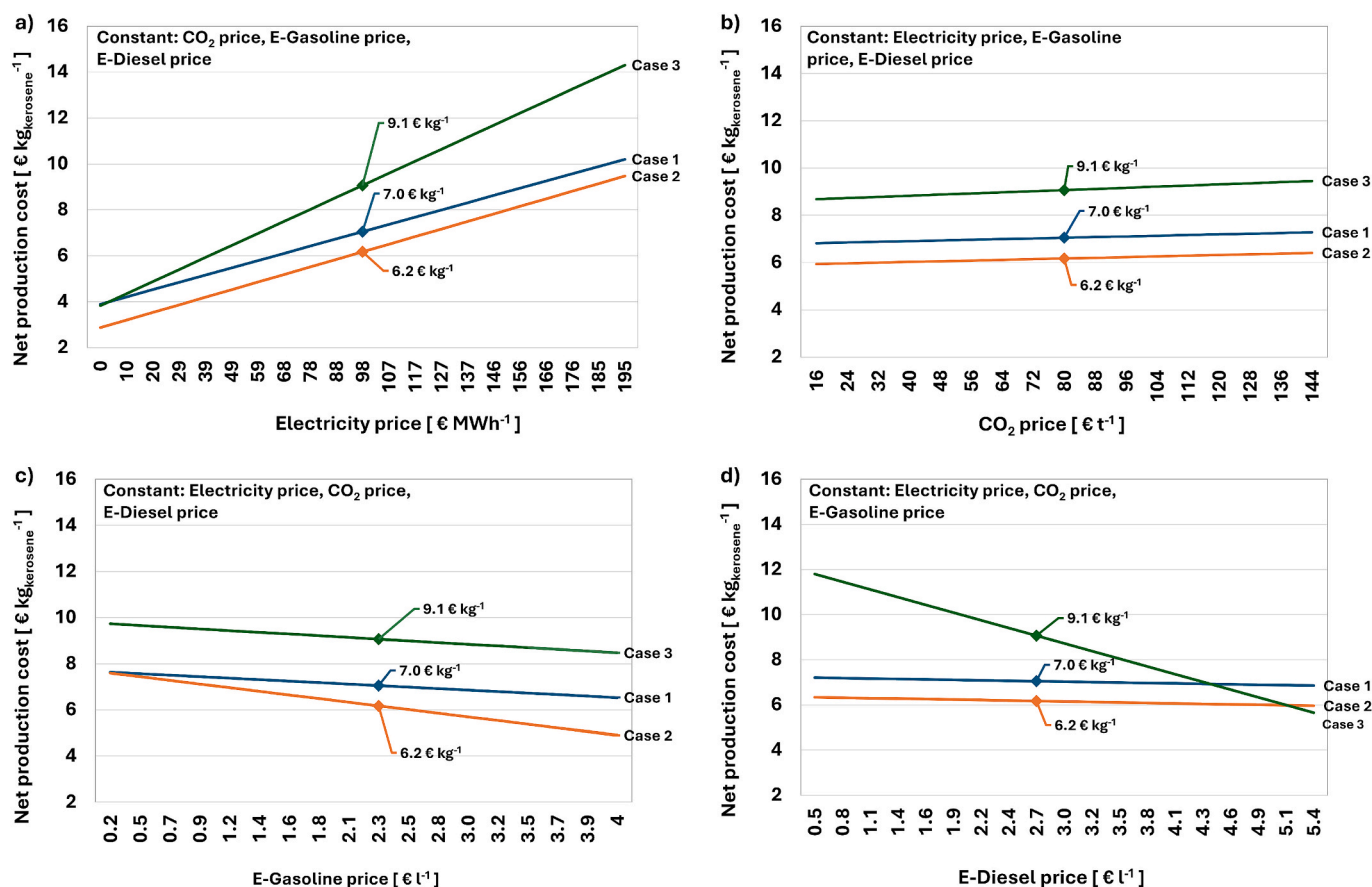


Fig. 9. Economic sensitivity analysis of raw material, utility and by-products prices: a) Electricity price, b) CO₂ price, c) e-gasoline price and, d) e-diesel price.

6. Conclusions

A maximum kerosene yield of 87.6 % and kerosene carbon efficiency of 86.9 % were achieved through the integrated optimization of FT synthesis and HC operating conditions, demonstrating that the PtL FT pathway can attain substantially higher kerosene yields than typically reported in the literature. The central advancement of this work is the coupling of detailed reaction kinetic models for both FT and HC within a complete process simulation framework. In contrast to studies that represent FT product distribution using a fixed chain-growth probability or treat upgrading as an isolated downstream step, this framework resolves the FT product spectrum as a function of temperature and H₂/CO ratio, and the hydrocracking as a function of temperature, pressure, and WHSV. This enables the direct evaluation of the combined influence of operating parameters on synthesis and upgrading of hydrocarbons. The integrated parameter study reveals that operating conditions maximizing liquid hydrocarbon production in the FT reactor do not necessarily maximize kerosene production after upgrading. Two competing constraints on kerosene yield were identified. Excessively severe FT operating conditions (230 °C, 25 bar, 2 H₂/CO molar ratio) promote the formation of light hydrocarbons, thereby increasing the recycle stream flow, whereas insufficient hydrocracking severity results in incomplete wax conversion and consequently alters the HC recycle hydrocarbon stream. Both effects act to reduce the overall kerosene yield, reinforcing the conclusion that optimal performance lies in the balanced configuration of FT and HC. Despite the improvement in kerosene yield, the PtL FT-kerosene remains energy intensive, exhibiting a Power-to-kerosene efficiency of 34.8 % and a hydrogen-to-kerosene efficiency of 69 %. The economic assessment further revealed that maximizing the kerosene yield does not necessarily minimize production cost. The kerosene net production cost ranged from 6.2 to 9.1 €₂₀₂₄ kg_{kerosene}⁻¹ review & editing, Software, Methodology. Nathanael Heimann:

across the representative cases, with the lowest cost achieved in Case 2 (with a 3 % lower kerosene yield offset by increased gasoline production, at an assumed e-gasoline price of 2.3 €₂₀₂₅ l⁻¹) rather than in the maximum kerosene yield case. Higher market value of by-products such as e-gasoline and e-diesel can improve the process economics through additional revenues. However, this advantage is realized only when their market prices exceed certain market values.

7. Outlook

FT synthesis remains a promising route for SAF production, demonstrated by its ability to achieve kerosene yield exceeding 85 %. Combined with its ASTM certified pathway, FT technology is well positioned to supply the blending mandates set under the ReFuelEU targets. However, this study relies on kinetic models taken from the literature, and there remains a need for validation of these findings in a demonstrator plant in order to substantiate them. Furthermore, advancements in FT and HC catalyst maturity is expected to improve both selectivity and energetic efficiency. For such a PtL FT plant, the optimal strategy will increasingly be governed by market dynamics rather than process design alone, since the economic viability of the plant depends significantly on the market value of by-products such as e-gasoline and e-diesel, which directly determine the most profitable product portfolio configuration.

CRedit authorship contribution statement

Mohammed Owais Khokar: Conceptualization, Methodology, Software, Data curation, Visualization, Writing – original draft. **Simil Shajan:** Visualization, Validation, Methodology. **Simon Maier:** Writing

Writing – review & editing, Visualization. **Ralph-Uwe Dietrich:** Writing – review & editing, Supervision, Resources, Funding acquisition.

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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuel.2026.141247>.

Data availability

Data will be made available on request.

References

- [1] European commission. The ReFuelEU Aviation SAF flexibility mechanism. 2025 27.2.2025; Available from: <https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=COM%3A2025%3A59%3AFIN>.
- [2] European Union Aviation Safety Agency (EASA). European Aviation Environmental Report 2025. 2025; Available from: <https://www.easa.europa.eu/en/domains/environment/eaer>.
- [3] International Air Transport Association. Available from IATA Annual Review 2024: 2024. <https://www.iata.org>.
- [4] European Parliament and Council of the European Union. Regulation (EU) 2023/2405 of the European Parliament and of the Council of 18 October 2023 on ensuring a level playing field for sustainable air transport (ReFuelEU Aviation). Available from Off J Eur Union October 2023;2023:31. <https://eur-lex.europa.eu/eli/reg/2023/2405/oj/eng>.
- [5] ASTM International. ASTM D7566-23a: Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons. 2023; Available from: <https://store.astm.org/d7566-23a.html>.
- [6] Adelung S, Dietrich R-U. Impact of the reverse water-gas shift operating conditions on the Power-to-Liquid fuel production cost. Fuel 2022;317. <https://doi.org/10.1016/j.fuel.2022.123440>.
- [7] Habermeyer F, et al. Power biomass to liquid — an option for Europe's sustainable and independent aviation fuel production. Biomass Convers Biorefin 2023;14(14): 16199–217. <https://doi.org/10.1007/s13399-022-03671-y>.
- [8] Todici B, et al. Kinetic modeling of secondary methane formation and 1-olefin hydrogenation in Fischer–Tropsch synthesis over a cobalt catalyst. Int J Chem Kinet 2017;49(12):859–74. <https://doi.org/10.1002/kin.21133>.
- [9] Ostadi M, Rytter E, Hillestad M. Boosting carbon efficiency of the biomass to liquid process with hydrogen from power: the effect of H₂/CO ratio to the Fischer–Tropsch reactors on the production and power consumption. Biomass Bioenergy 2019;127. <https://doi.org/10.1016/j.biombioe.2019.105282>.
- [10] Eyberg V, et al. Techno-economic assessment and comparison of Fischer–Tropsch and methanol-to-Jet processes to produce sustainable aviation fuel via power-to-liquid. Energ Conver Manage 2024;315. <https://doi.org/10.1016/j.enconman.2024.118728>.
- [11] Kirsch H, et al. Power-to-fuel conversion based on reverse water-gas-shift, Fischer–Tropsch synthesis and hydrocracking: mathematical modeling and simulation in matlab/simulink. Chem Eng Sci 2020;227. <https://doi.org/10.1016/j.ces.2020.115930>.
- [12] Bube S, et al. Kerosene production from power-based syngas – a technical comparison of the Fischer–Tropsch and methanol pathway. Fuel 2024;366:131269. <https://doi.org/10.1016/j.fuel.2024.131269>.
- [13] Gambaro C, et al. Hydrocracking of Fischer–Tropsch waxes: kinetic modeling via LHHW approach. AIChE J 2011;57(3):711–23. <https://doi.org/10.1002/aic.12291>.
- [14] Finlayson BA. Equation of state.. Available from: Introduction to Chemical Engineering Computing 2012;7–28. <https://onlinelibrary.wiley.com/doi/abs/10.1002/9781118309599.ch2>.
- [15] Heimann N, et al. Comparable techno economic- and life-cycle assessment of PtX production at offshore locations. Manuscript in preparation 2026.
- [16] Adelung S, Maier S, Dietrich R-U. Impact of the reverse water-gas shift operating conditions on the power-to-liquid process efficiency. Sustainable Energy Technol Assess 2021;43. <https://doi.org/10.1016/j.seta.2020.100897>.
- [17] de Klerk, A. Chapter 10 - Aviation Turbine Fuels Through the Fischer–Tropsch Process. Biofuels for Aviation 2016; 241–259. Available from: <https://www.sciencedirect.com/science/article/pii/B978012804568800010X>.
- [18] Iglesia E. Design, synthesis, and use of cobalt-based Fischer–Tropsch synthesis catalysts. Appl Catal A 1997;161(1):59–78. [https://doi.org/10.1016/S0926-860X\(97\)00186-5](https://doi.org/10.1016/S0926-860X(97)00186-5).
- [19] Todici B, et al. CO-insertion mechanism based kinetic model of the Fischer–Tropsch synthesis reaction over re-promoted Co catalyst. Catal Today 2014;228:32–9. <https://doi.org/10.1016/j.cattod.2013.08.008>.
- [20] Habermeyer F, et al. Sustainable aviation fuel from forestry residue and hydrogen – a techno-economic and environmental analysis for an immediate deployment of the PBT process in Europe. Sustainable Energy Fuels 2023;7(17):4229–46. <https://doi.org/10.1039/D3SE00358B>.
- [21] LeViness S, et al. Velocys Fischer–Tropsch synthesis technology—new advances on state-of-the-art. Top Catal 2013;57(6–9):518–25. <https://doi.org/10.1007/s11244-013-0208-x>.
- [22] Rytter E, Holmen A. Perspectives on the effect of water in cobalt Fischer–Tropsch synthesis. ACS Catal 2017;7(8):5321–8. <https://doi.org/10.1021/acscatal.7b01525>.
- [23] Habermeyer F, et al. Techno-economic analysis of a flexible process concept for the production of transport fuels and heat from biomass and renewable electricity. Front Energy Res 2021;9. <https://doi.org/10.3389/fenrg.2021.723774>.
- [24] Gamba S, et al. introduction of a breakage probability function in the hydrocracking reactor model. Ind Eng Chem Res 2009;48(12):5656–65. <https://doi.org/10.1021/ie8019455>.
- [25] Maryland Department of the Environment. Md. Code Regs. 03.03.05.02 - Specifications for No. 1-D and No. 2-D Diesel Fuel (ASTM D-975). Available from: <https://www.law.cornell.edu/regulations/maryland/COMAR-03-03-05-02>.
- [26] Shell Trading Canada. Safety Data Sheet: Premium Unleaded Gasoline 2025; Available from: <https://www.epc.shell.com/DocumentManagement/BlobDocumentDownload?DocId=92233318>.
- [27] Klerk, A.d. Cracking. Fischer–Tropsch Refining 2011;407–440. Available from: doi: 10.1002/9783527635603.ch21.
- [28] Nyholm F, Toppinen S, Saxén H. Sustainable power-to-liquids aviation fuels: modelling and comparison of two Fischer–Tropsch upgrading process concepts. Energ Conver Manage 2025;342. <https://doi.org/10.1016/j.enconman.2025.120153>.
- [29] Maier S, Weyand J, Pyteea - a Python-based toolbox for automated technical, economic and environmental. Assessment 2025.
- [30] Rahmat Y, et al. Techno-economic and exergy analysis of e-methanol production under fixed operating conditions in Germany. Appl Energy 2023;351. <https://doi.org/10.1016/j.apenergy.2023.121738>.
- [31] Heimann N, et al. Contribution to a standardized economic and ecological assessment methodology for e-fuel production in Germany. Front Energy Res 2025; 13. <https://doi.org/10.3389/fenrg.2025.1297299>.
- [32] Peters MS, Timmerhaus KD, West RE, Plant Design and Economics for Chemical Engineers. 2004, McGraw-Hill.
- [33] Albrecht FG, et al. A standardized methodology for the techno-economic evaluation of alternative fuels – a case study. Fuel 2017;194:511–26. <https://doi.org/10.1016/j.fuel.2016.12.003>.
- [34] AACE International. Cost Estimate Classification System - as Applied in Engineering, Procurement, and Construction for the Process Industries. 2011 [cited 2011]; Available from: <https://web.aacei.org/>.
- [35] European Environment Agency. Share of renewable energy in final energy consumption. 2025; Available from: <https://www.eea.europa.eu/en/europe-environment-2025/countries/norway/renewable-energy-sources>.
- [36] AG, A.G. Norway implements the EU's ReFuelEU Aviation regulations. 2025; Available from: <https://aither.com/update/norway-implements-the-eus-refueu-aviation-regulations>.
- [37] Everson N, et al. What is the potential of bioCCS to deliver negative emissions in Norway? From biomass mapping to a window of negative emissions potential. Sustain Mater Technol 2024;40:e00912. <https://doi.org/10.1016/j.susmat.2024.e00912>.
- [38] Schemme S, et al. H₂-based synthetic fuels: a techno-economic comparison of alcohol, ether and hydrocarbon production. Int J Hydrogen Energy 2020;45(8): 5395–414. <https://doi.org/10.1016/j.ijhydene.2019.05.028>.
- [39] Schorn F, et al. Methanol as a renewable energy carrier: an assessment of production and transportation costs for selected global locations. Adv Appl Energy 2021;3:100050. <https://doi.org/10.1016/j.adapen.2021.100050>.
- [40] Krämer SM, et al. Power- and biomass-to-liquid processes with fuel-assisted solid oxide electrolysis cells and water gas shift-adjusted systems: a techno-economic analysis. Fuel 2025;396. <https://doi.org/10.1016/j.fuel.2025.135290>.
- [41] Eurostat. Electricity prices for non-household consumers (nrg_pc_205). 2026; Available from: https://ec.europa.eu/eurostat/databrowser/product/page/NRG_PC_205.
- [42] Eurostat. Labour cost, wages and salaries, direct remuneration (excluding apprentices) by NACE Rev. 2 activity (lc_ncost_r2). Available from: https://ec.europa.eu/eurostat/databrowser/view/lc_ncost_r2_custom_21123741/default/table.
- [43] Frontier Economics. Szenarien für den Markthochlauf von E-Fuels im Straßenverkehr. 2024; Available from: https://www.efuel-alliance.eu/fileadmin/Downloads/Frontier_Economics_-_Szenarien_fu%CC%88r_Markthochlauf_von_E-Fuels_im_Stra%C3%9Fenverkehr_24_.pdf.
- [44] Ma W-P, et al. An investigation of chain growth probability in Fischer–Tropsch synthesis over an industrial Fe–Cu–K catalyst. React Kinet Catal Lett 1999;66(2): 217–23. <https://doi.org/10.1007/BF02475793>.