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Chike Ucheana

cnucheana2@sheffield.ac.uk

University of Sheffield

Maria Fernanda Rojas-Michaga

University of Sheffield

Kevin J. Hughes

University of Sheffield

Derek Ingham

University of Sheffield

Mohamed Pourkashanian

University of Sheffield

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A Techno-Economic, Environmental and Social Life Cycle Assessments of Sustainable Aviation Fuel production via the Alcohol-to-Jet process – A UK Case Study

**Chike Ucheana^{a,1}, Maria Fernanda Rojas-Michaga^a, Kevin J. Hughes^a, Derek Ingham^a,
Mohamed Pourkashanian^a**

^a*Energy 2050, School of Mechanical, Aerospace and Civil Engineering, University of Sheffield, Sheffield,
United Kingdom*

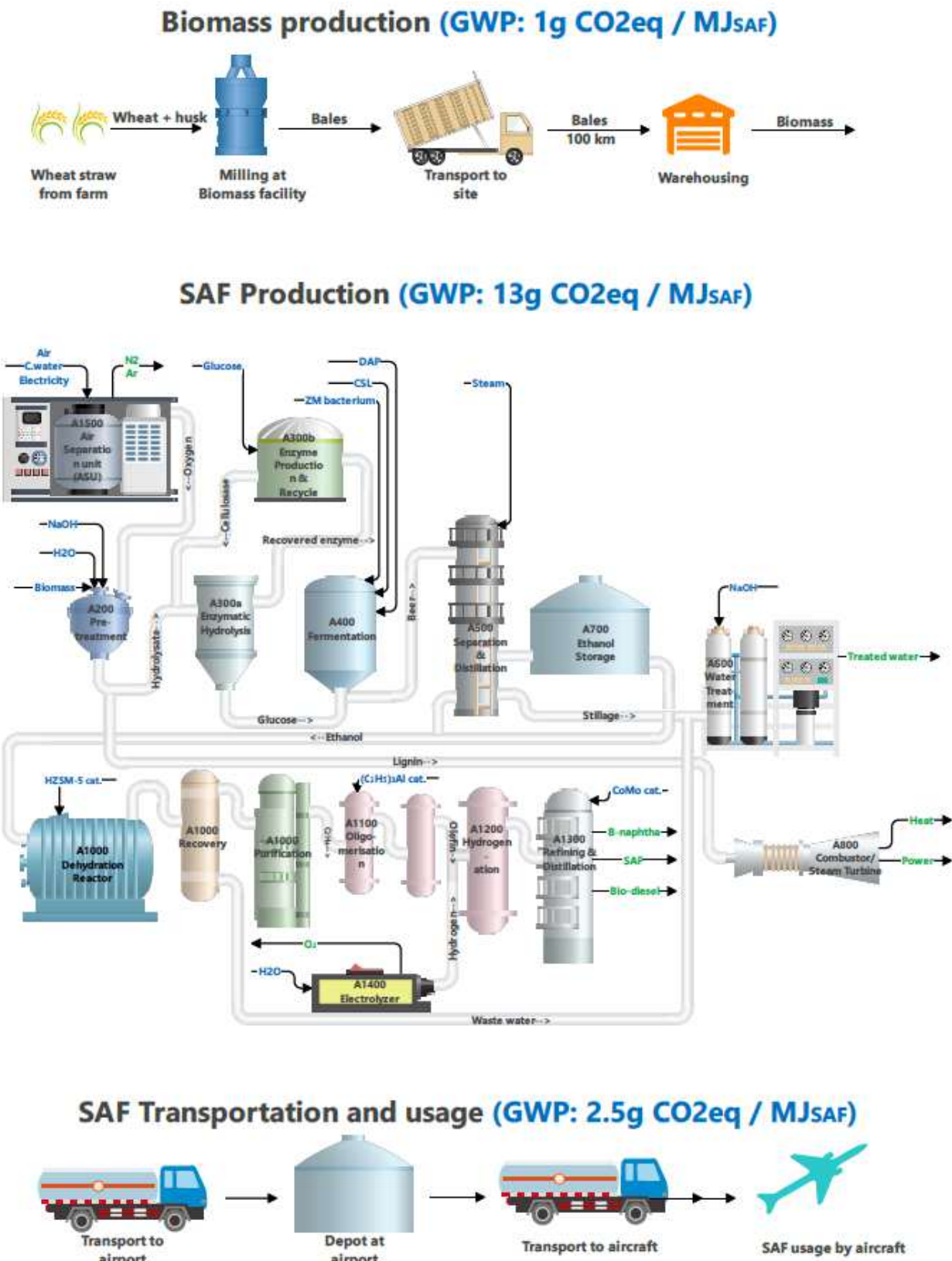
¹*Corresponding author: email address: cnucheana2@sheffield.ac.uk*

Abstract

This study presents a multi-dimensional (techno-economic, environmental, and social life cycle) assessment of sustainable aviation fuel production via the alcohol-to-jet pathway using lignocellulosic wheat straw and UK as a case study. A self-sufficient, integrated biorefinery was modelled in Aspen Plus®, incorporating in situ hydrogen and oxygen generation, enzyme production, co-product recovery (bio-naphtha, biodiesel), and waste-to-energy cogeneration. A techno-economic analysis was performed through discounted cash flow modelling, while environmental and social impacts were evaluated using ISO 14040/44-compliant life cycle assessment and PSILCA-based social life cycle assessment. Thermodynamic results indicate overall biomass-to-product conversion efficiency of 11% with 68% SAF selectivity, with >90% residue valorisation through a 66 MW Rankine-cycle cogeneration unit, enabling full internal energy supply and 48 MW of net electricity export. The economic analysis estimates capital and operating costs of £475 M and £193 M, with annual co-product revenues of £140 M. The Minimum

21 Jet Fuel Selling Price ranges between £0.75 - £4.53/kg, strongly dependent on policy incentives
22 and equity structure. Environmental assessment results show up to 80% greenhouse gas
23 reduction compared to fossil jet comparator, while S-LCA highlights road transport and SAF
24 production as the highest social risk sectors, with “fair salary” as the most critical indicator.
25 Sensitivity and Monte Carlo analyses identify feedstock, enzymes, and utilities as dominant
26 economic drivers, while scale-up from 1,000 to 4,000 t/day reduces MJSP substantially. Overall,
27 the AtJ pathway demonstrates high SAF selectivity >70% and resource integration, offering strong
28 potential for aviation decarbonisation under supportive policy and regulatory frameworks.

29 Graphic Abstract



30
31

32 **Nomenclature**

33 **Abbreviations**

34	AEL	Alkaline Electrolyzer
35	ASU	Air Separation Unit
36	Aspen Plus®	Process simulation software developed by Aspen Technology, Inc.
37	ASTM	American Society for Testing and Materials
38	AtJ	Alcohol-to-Jet
39	CAPEX	Capital Expenditure
40	CEPCI	Chemical Engineering Plant Cost Index
41	CfD	Contracts for Difference
42	CHP	Combined Heat and Power
43	CO ₂	Carbon Dioxide
44	CO ₂ eq	Carbon Dioxide Equivalent
45	CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
46	CRedit	Contributor Roles Taxonomy
47	CSL	Corn Steep Liquor
48	DAP	Diammonium Phosphate
49	DAC	Direct Air Capture
50	DCFA	Discounted Cash Flow Analysis
51	DM	Dry Matter
52	EIC	Energy Innovation Centre
53	E-LCA	Environmental Life Cycle Assessment
54	EPCM	Engineering, Procurement and Construction Management
55	EURO6	Euro 6 vehicle emissions standard

56	FCI	Fixed Capital Investment
57	FOAK	First-of-a-Kind
58	FOC	Fixed Operating Cost
59	FOM	Fixed Operating & Maintenance (costs)
60	GBR	United Kingdom
61	GHG	Greenhouse Gas
62	GJ	Gigajoule
63	GVA	Gross Value Added
64	GWP	Global Warming Potential
65	HZSM-5	Zeolite catalyst
66	IC	Indirect Costs
67	IDC	Installed Direct Costs
68	ILUC	Indirect Land Use Change
69	ILUC	Indirect Land Use Change
70	IPCC	Intergovernmental Panel on Climate Change
71	IRR	Internal Rate of Return
72	ISO	International Organization for Standardization
73	Jet A-1	Standard petroleum aviation kerosene
74	LCA	Life Cycle Assessment
75	LHV	Lower Heating Value
76	MJSP	Minimum Jet Fuel Selling Price
77	MRIO	Multi-Regional Input–Output
78	mrh	Medium Risk Hours
79	NaOH	Sodium Hydroxide
80	NIDC	Non-Installed Direct Costs
81	NOAK	Nth-of-a-Kind

82	NPT	Nova Pangaea Technologies
83	NPV	Net Present Value
84	NREL	National Renewable Energy Laboratory
85	OHS	Occupational Health and Safety
86	OPEX	Operating Expenditure
87	PEC	Purchased Equipment Cost
88	PSILCA	Product Social Impact Life Cycle Assessment (database)
89	QGIS	Quantum Geographic Information System
90	RCM	Renewable and Clean Mandate
91	RTFO	Renewable Transport Fuel Obligation
92	S-LCA	Social Life Cycle Assessment
93	SAF	Sustainable Aviation Fuel
94	SCL	Sodium Citrate Liquor
95	SDGs	Sustainable Development Goals
96	SIA	Social Impact Assessment
97	TCI	Total Capital Investment
98	TDC	Total Direct Costs
99	UK	United Kingdom
100	UNFCCC	United Nations Framework Convention on Climate Change
101	USA	United States of America
102	USD	United States Dollar
103	VOC	Variable Operating Cost
104	WC	Working Capital
105	WHSV	Weight Hourly Space Velocity
106	WtWa	Well-to-Wake (cradle-to-grave)
107		

108 **Symbols and Units**

109 **Energy & Power Units**

110	kWh	Kilowatt-hour (3.6×10^6 joules)
111	MJ	Megajoule (10^6 joules)
112	MJ/kg	Megajoules per kilogram
113	MM	Million (10^6)
114	MMT	Million Metric Tonnes
115	MW	Megawatt (10^6 watts)
116	MWh	Megawatt-hour
117	MW _e	Megawatt-electric (unit of electric power)
118	MW _t	Megawatt-thermal (unit of thermal power)
119	TJ	Terajoule

120 **Mass & Flow Units**

121	T	Metric tonne (1,000 kg)
122	kg	Kilogram
123	g	Gram
124	t/h	Tonne per hour
125	kg/h	Kilogram per hour
126	kg/s	Kilogram per second
127	g/h	Gram per hour
128	g/L	Grams per litre
129	wt%	Weight percent

130 **Economic Units**

131	£/t	Pounds per tonne
132	£/MJ	Pounds per megajoule

133	£/GJ	Pounds per gigajoule
134	£/bbl	Pounds per barrel
135	MM£	Million Pounds
136	£	Pounds
137	<u>Environmental & Emissions Units</u>	
138	g CO ₂ eq/MJ	Grams of CO ₂ equivalent per megajoule
139	kg CO ₂ eq/t	Kilograms of CO ₂ equivalent per tonne
140	t CO ₂ eq/year	Tonnes of CO ₂ equivalent per year
141	<u>Thermodynamic & Process Variables</u>	
142	η	Efficiency (dimensionless, %)
143	T	Temperature (°C or K)
144	P	Pressure (bar, MPa, Pa)
145	ΔH	Enthalpy change (kJ/mol or MJ/kg)
146	ΔS	Entropy change (kJ/mol·K)
147	$\dot{m}$	Mass flow rate (kg/h, kg/s, or t/h)
148	$\dot{V}$	Volumetric flow rate (m ³ /h or m ³ /s)
149	<u>Physical & Volume Units</u>	
150	m ³	Cubic metre
151	m ³ /h	Cubic metre per hour
152	L	Litre
153	L/h	Litre per hour
154	<u>Other Symbols</u>	
155	R	Ideal gas constant (8.314 J/mol·K)
156	Y	Yield (dimensionless, %)
157		

1.0 Introduction

The decarbonization of the global aviation sector is essential to achieving climate targets, particularly as aviation accounts for approximately 2.5% of global CO₂ emissions and its energy demand is projected to triple by 2050 [1]. Unlike other transport sectors, aviation remains dependent on high energy-density liquid fuels, with limited prospects for large-scale electrification of long-haul flights. Consequently, Sustainable Aviation Fuels (SAFs) have emerged as one of the most promising near- to medium-term decarbonisation solutions, offering lifecycle greenhouse gas (GHG) emission reductions of up to 80% relative to conventional Jet A [2, 3]. However, widespread SAF deployment remains constrained by high production costs, uncertain feedstock supply chains, limited commercial-scale implementation, and insufficient understanding of system-level sustainability trade-offs.

Among the approved SAF pathways, the Alcohol-to-Jet (AtJ) process converts bioethanol into drop-in aviation fuel through dehydration, oligomerisation, and hydrogenation. Tao et al. [4] demonstrated that ethanol-to-jet upgrading can achieve substantial cost reductions under optimised operating conditions, while Geleynse et al. [5] confirmed the technical viability of the AtJ pathway and its compliance with ASTM D7566 fuel specifications. Nevertheless, these studies focused primarily on fuel upgrading and did not evaluate fully integrated biorefineries or broader sustainability dimensions, including social impacts and regional development.

Lignocellulosic biomass, particularly wheat straw, is an attractive second-generation feedstock because it avoids food-versus-fuel competition while valorising agricultural residues [6]. Integrating such feedstocks within biorefineries promotes circular resource utilisation through waste recovery and combined heat and power (CHP) generation [7]. Furthermore, integrating

hydrolysis, fermentation, catalytic upgrading, and multi-stage Rankine-cycle CHP systems can significantly improve energy efficiency and reduce fossil energy demand [8].

Although second-generation ethanol production has been extensively investigated, particularly through National Renewable Energy Laboratory (NREL) developments, the subsequent upgrading of lignocellulosic ethanol to SAF via the AtJ pathway remains comparatively underexplored [4]. Existing studies have largely focused on isolated process stages rather than integrated system performance. Tao et al. [4] evaluated ethanol-to-jet upgrading economics, Klein et al. [9] combined techno-economic and environmental assessments for Brazilian sugarcane biorefineries, Geleynse et al. [5] assessed the AtJ conversion pathway, Crawford et al. [10] analysed poplar-based biojet production, and Atsonios et al. [11] compared advanced thermochemical e-kerosene pathways. While these studies significantly advanced understanding of SAF production, they generally considered either ethanol production or fuel upgrading independently and rarely evaluated the interactions between process integration, mass and energy integration, utility self-sufficiency, and overall sustainability.

Similarly, Calderon [12] investigated enzyme recycling for lignocellulosic ethanol production, Humbird et al. [13] established the benchmark Aspen Plus® model for biochemical ethanol production, and Kazi et al. [14] compared alternative biochemical conversion technologies. However, the absence of integrated process modelling limits the assessment of how process configuration, energy integration, and utility self-sufficiency influence overall techno-economic and sustainability performance [15, 16].

Environmental assessments have also remained relatively narrow. Michailos [17] combined techno-economic analysis with life cycle assessment (LCA) for jet fuel production from sugarcane residues, while Vela-García et al. [18] evaluated triisobutane biojet fuel using TEA and LCA. Nevertheless, most studies focus primarily on greenhouse gas emissions and rarely

consider wider environmental indicators, such as water use, land use change, or biodiversity. More importantly, social sustainability remains largely neglected despite constituting one of the three pillars of sustainable development [19].

The adoption of the United Nations Sustainable Development Goals (SDGs) has further highlighted the need to integrate environmental, economic, and social dimensions across increasingly complex global supply chains [20, 21]. Although Social Life Cycle Assessment (S-LCA) provides a systematic framework for evaluating social risks, existing SAF studies are largely limited to qualitative assessments or simple employment metrics [22, 23]. While Wang et al. [24, 25], explored social sustainability within aviation biofuel supply chains, no study has yet applied process-level S-LCA to the AtJ pathway using the internationally recognised PSILCA database.

To address these knowledge gaps, this study presents the first fully integrated assessment of Sustainable Aviation Fuel production via the Alcohol-to-Jet pathway from lignocellulosic wheat straw within a UK context. A self-sufficient Aspen Plus® biorefinery incorporating alkaline oxidative pretreatment, enzymatic hydrolysis, fermentation, ethanol upgrading, in situ hydrogen, oxygen and enzyme production, co-product recovery (bio-naphtha and biodiesel), and a 66 MW three-pressure Rankine-cycle cogeneration system was developed. The integrated system achieves full internal energy self-sufficiency with net electricity export and is evaluated through discounted cash flow analysis, ISO 14040/44-compliant environmental life cycle assessment implemented in SimaPro [26] and PSILCA-based social life cycle assessment using UK-specific indicators.

This study tests the hypothesis that a fully integrated lignocellulosic AtJ biorefinery can achieve technical feasibility, economic competitiveness, and net sustainability benefits when energy self-sufficiency and co-product valorisation are incorporated. By linking rigorous process modelling with techno-economic, environmental, and social assessments, the work identifies

critical cost drivers, environmental hotspots, and social risks while providing optimisation pathways for technology developers and policymakers. The findings align with the UK SAF Mandate and RefuelEU Aviation targets [27], providing a scalable framework for advancing low-carbon aviation fuel production in support of global decarbonisation goals.

In summary, as detailed in **Table 1**, existing literature shows three critical gaps:

- (i) absence of fully integrated Aspen-based AtJ plant models,
- (ii) lack of combined TEA–E-LCA–S-LCA frameworks, and
- (iii) no UK-specific residue-based AtJ case studies aligned with policy.

This study tests the hypothesis that a fully integrated lignocellulosic AtJ biorefinery can achieve technical feasibility, economic competitiveness, and net sustainability benefits when energy self-sufficiency and co-product valorisation are incorporated.

Table 1. Benchmark with peer-reviewed studies

Study (year)	Relevance	Integrated ethanol + upgrading to SAF	TEA	E-LCA	S-LCA	Energy self-sufficient design	UK-based
Falter et al. (2020) [23]	One of the clearest tri-pillar (TEA+E-LCA+S-LCA) quantitative assessments; strong sustainability framework precedent	×	✓	✓	✓	×	×
Rojas-Michaga et al. (2023) [28]	Combined TEA + LCA for SAF (PtL) with strong system boundary treatment (methodological comparator for	×	✓	✓	×	●	✓

	TEA/LCA integration)						
Anekwe et al. (2024) [29]	Recent TEA + life-cycle analysis for bioethanol-to-hydrocarbon fuel blend stocks; good modern comparator for upgrading performance/cost	●	✓	✓	×	×	×
Michailos (2018)	Process design + economic evaluation + LCA for jet fuel from biomass residue (close in “residue-to-jet” framing)	●	✓	✓	×	●	×
Klein et al. (2018)	Integrated biorefinery with TEA + E-LCA for renewable jet fuel in a regional context (Brazil sugarcane)	●	✓	✓	×	●	×
Han, Tao & Wang (2017)	Strong well-to-wake comparison of EtJ/S2J pathways; good GHG accounting reference	×	×/●	✓	×	×	×
Geleynse et al. (2018)	Clear AtJ pathway TEA; useful pathway economics comparator	●	✓	×	×	×	×
Tao et al. (2017)	Detailed TEA of upgrading ethanol-to-jet blend stocks, cost drivers for upgrading block	●	✓	×	×	×	×
UK comparator: ICF (2023)	UK deployment context: feedstock supply,	●	●	●	×	×	✓

UK Sustainable Aviation SAF Roadmap (report)	logistics constraints, policy/market pathways (useful to justify UK assumptions; not peer-reviewed)						
This study (2026)	Fully integrated Aspen model (wheat straw → ethanol → AtJ upgrading) + TEA + E-LCA + S-LCA + Energy self-sufficiency + UK case	✓	✓	✓	✓	✓	✓

Legend: ✓ = explicitly covered; ● = partially/indirectly covered; ✕ = not covered / not the focus

2.0 Methods

The overall methodological framework adopted in this study is illustrated in **Figure 1**. The investigation comprises six sequential stages. Stage 1 identifies the most suitable lignocellulosic feedstock for Sustainable Aviation Fuel (SAF) production within the UK context. Stage 2 evaluates candidate pretreatment and conversion technologies and establishes the selected biomass-to-ethanol-to-jet (AtJ) process configuration. Stages 3–6 assess the selected biorefinery through integrated thermodynamic process modelling, techno-economic analysis (TEA), environmental life cycle assessment (E-LCA), and social life cycle assessment (S-LCA), respectively. The thermodynamic process model developed in Aspen Plus® forms the basis for the economic, environmental, and social assessments by providing the mass and energy balances required for each evaluation. The methodology adopted for each stage is described in the following sections.

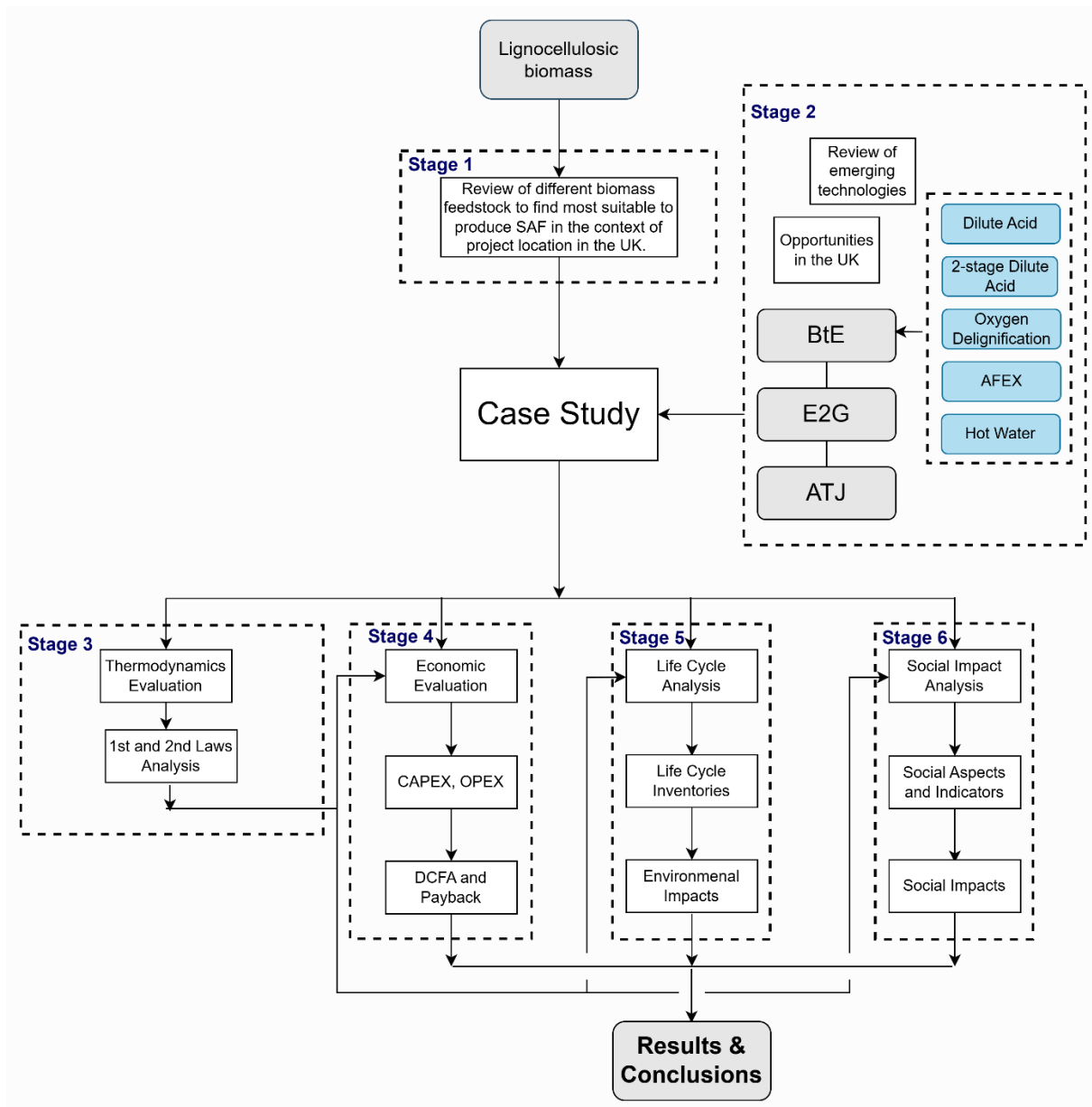


Figure 1. Methodology flowchart

2.1 Feedstock selection

The feedstock selection was undertaken by screening major UK biomass resources, including agricultural residues, forestry by-products, and waste oils, against feedstock availability, sustainability, and policy requirements. As feedstock cost is a dominant contributor to biorefinery economics [13, 30], UK policy prioritises wastes and agricultural residues while prohibiting the use of dedicated cropland for biofuel production [31]. Consequently, crop-

derived fuels are ineligible under the UK SAF Mandate, making agricultural and forestry residues the preferred feedstocks for Sustainable Aviation Fuel (SAF) production [32].

The UK has approximately 4.6 million hectares of arable land, with wheat (1.72 Mha) and barley (1.14 Mha) representing the dominant cereal crops in 2023 [33]. These produced an estimated 9.7 Mt of cereal straw [33]. Based on straw-to-grain ratios of 76% for wheat and 82% for barley, the theoretical annual production is approximately 10.7 Mt of wheat straw and 5.8 Mt of barley straw [33]. However, maintaining soil health requires a substantial fraction of straw to remain on the field, reducing the practically recoverable resource to approximately 2-5 Mt/year [34]. By comparison, forest residues are estimated to supply less than 2 Mt/year, while used cooking oil could satisfy only 0.3-0.6% of UK jet fuel demand [34] (about 0.2 Mt fuel) and used cooking oil provides only 0.3 - 0.6% of jet fuel demand [34]. Wheat straw therefore represents the largest and most sustainable domestic lignocellulosic resource for the Alcohol-to-Jet (AtJ) pathway.

Wheat straw was selected as the base-case feedstock because of its high availability, low cost, favourable cellulose content for ethanol production, and alignment with UK Department for Transport (DfT) sustainability requirements, which prioritise agricultural residues that avoid dedicated cropland and food-versus-fuel competition [32]. In addition, the lignin-rich residue provides an opportunity for energy recovery, improving overall resource efficiency and supporting circular economy objectives.

The proposed biorefinery processes 2,000 t/day (2,200 U.S. tons/day) of wheat straw, consistent with the benchmark National Renewable Energy Laboratory (NREL) cellulosic biorefinery design [13]. Continuous operation at 8,400 h/year requires approximately 770,000 t/year of straw, corresponding to about 121,000 ha of wheat cultivation at typical straw yields of 7-8 t/ha [33]. This represents approximately 7-8% of the UK's wheat-growing area and can be achieved without affecting grain production, as straw is recovered as an agricultural residue during harvesting. The

proposed system therefore supports simultaneous food and fuel production while remaining consistent with UK circular economy and SAF sustainability objectives.

2.2 Biorefinery design configuration

The biorefinery is designed around three objectives: (i) integration of biochemical ethanol production with downstream Sustainable Aviation Fuel (SAF) upgrading to minimise transport and logistics; (ii) energy and utility self-sufficiency through on-site power, hydrogen, and oxygen generation; and (iii) co-product valorisation. The co-located facility is envisaged in southeast England, near feedstock supplies and transport infrastructure. Wheat straw (2,000 t/day) undergoes alkaline oxidative pretreatment using dilute NaOH and oxygen to remove lignin and disrupt the biomass structure under mild conditions [12] followed by enzymatic hydrolysis and fermentation. Consistent with the NREL design [13], cellulase is produced on-site to reduce enzyme supply and cost uncertainties. The resulting ethanol is purified by distillation and molecular sieves to approximately 21,000 kg/h of anhydrous ethanol before Alcohol-to-Jet (AtJ) upgrading through dehydration to ethylene, oligomerisation to higher olefins, and hydrogenation to saturated jet-range hydrocarbons. The overall process configuration is shown in **Figure 2**.

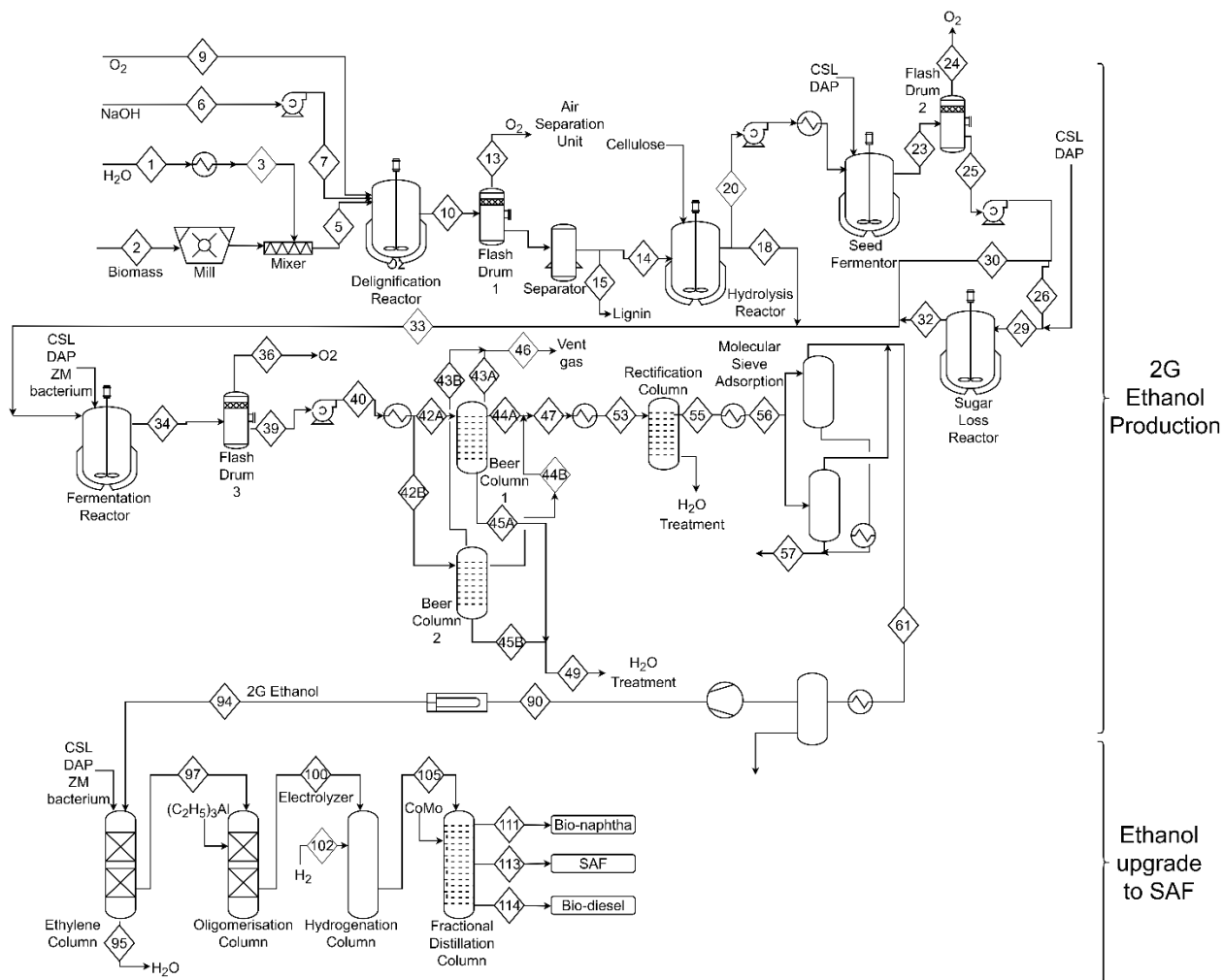


Figure 2. Simplified Process Flow Diagram of the AtJ Production (with Aspen stream numbers)

Renewable hydrogen for upgrading is generated by an on-site alkaline electrolyzer, which simultaneously produces oxygen ([35]. Part of this oxygen is used for oxidative pretreatment, while an air separation unit (ASU) supplies additional oxygen for pretreatment and combustion and produces nitrogen for inerting or sale. Lignin-rich solid residues and unconverted carbohydrates are combusted to generate process steam and drive a three-stage Rankine-cycle cogeneration system producing 66 MW of gross electricity. Approximately 18 MW is consumed internally, including the electrolyzer and other process loads, leaving 48 MW for grid export. Wastewater is treated and recycled where practicable, consistent with the NREL design

incorporating stillage and inorganic handling [13]. This integrated configuration therefore reduces external utility requirements while valorising residual biomass and surplus energy and gases.

The selected capacity is consistent with established biorefinery designs. Humbird et al. [13] modelled an NREL nth-plant facility processing 2,205 t/day, while Kazi et al. [14] evaluated a 2,200 t/day corn-stover ethanol facility. Huang et al. [36]. similarly demonstrated substantial reductions in ethanol production cost as capacity increased from 1,000 to 2,000 t/day, supporting the selected 2,000 t/day design basis. The present configuration extends these benchmark designs by integrating AtJ upgrading with on-site hydrogen, oxygen and electricity generation to improve resource integration and plant self-sufficiency.

2.3 Process modelling approach

The integrated SAF process was simulated in Aspen Plus® v14 using the experimental-based pretreatment data of Calderon [12] and the NREL biomass-to-ethanol design [13], as modelling benchmarks, with downstream AtJ upgrading incorporated following Tao et al. [4]. Prior to scale-up, the pretreatment model was validated against Calderon's Scenario S20-5 [12]. with deviations below 1% for major component mass flowrates; the validation model and detailed comparison are provided in **Supplementary Material A4.0**.

Figure 3 presents the integrated process configuration linking biomass conversion, ethanol production, AtJ upgrading, and supporting utility systems. Process-area mass and energy balances were established in **Table 8** and heat integration was evaluated using Aspen Energy Analyzer [13]. Detailed unit-operation specifications are provided in the **Supplementary material A2.2**.

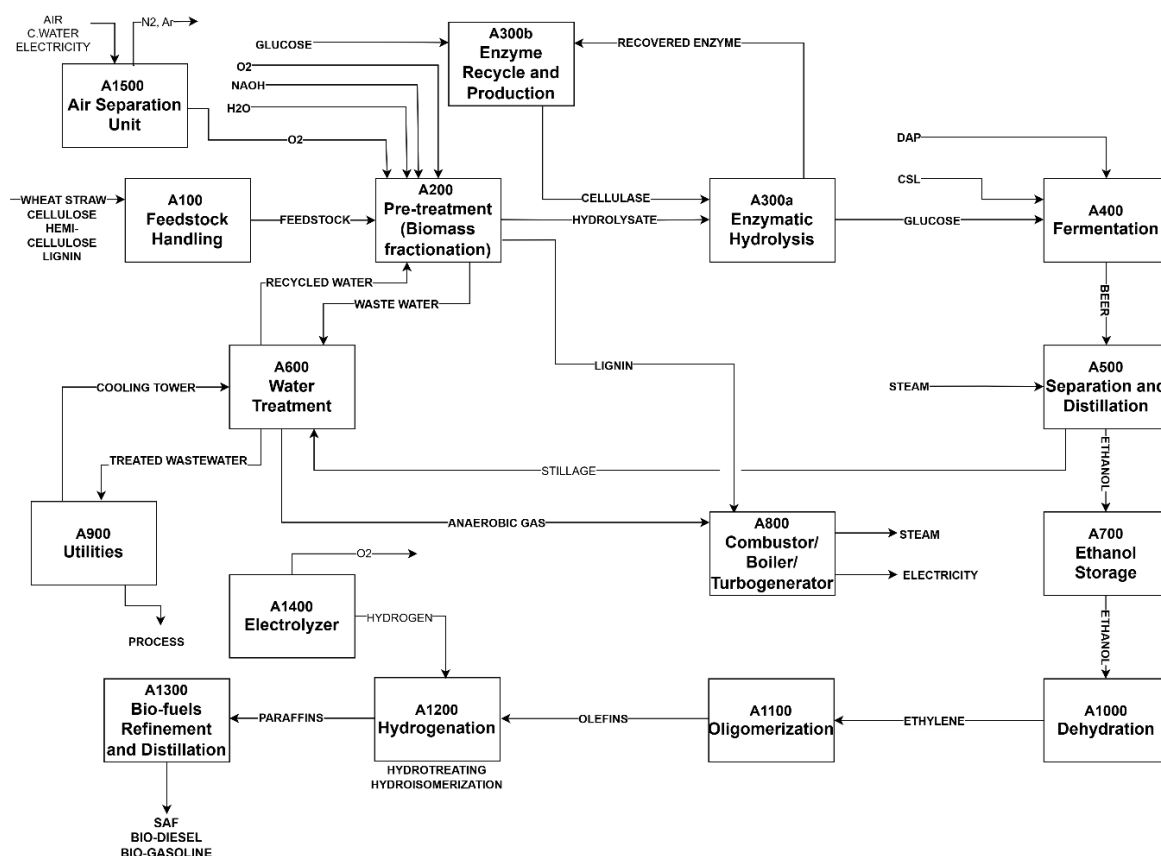


Figure 3. Overall Block Flow Diagram of the Biorefinery

Model fidelity was additionally assessed against independent peer-reviewed benchmarks for key AtJ conversion stages in **Table 2**. The principal deviation was the simulated ethylene yield of 90% compared with the literature value of 98.8%, reflecting conservative conversion assumptions and explicit representation of DEE and light-olefin by-products.

Table 2. Validation of Aspen Plus® model outputs against literature benchmarks

Parameter	Literature benchmark (%)	Aspen model output (%)	% deviation	Reference
Ethanol dehydration conversion	99.9	100	+0.1	Kagyrmannova et al. [37]
Ethylene yield	98.8	90	-8.9	Mohsenzadeh et al. [38]
SAF selectivity	70	70	0	Geleynse et al. [5]

2.4 Thermodynamics Performance Indicators

Thermodynamic performance was evaluated using mass, energy, and exergy balances. First-law analysis was used to determine feedstock conversion, energy efficiency, and net electricity production, while second-law analysis quantified exergetic efficiency and process irreversibility. The following performance indicators were applied.

i. *Carbon conversion efficiency* (η_c) is an indicator that measures the extent to which feedstock is converted into the desired product. This efficiency is quantified using **Equation 1**, which correlates the moles of carbon ($\dot{n}_{c_{Products}}$ in kmol/h) present in the products with the moles of carbon ($\dot{n}_{c_{feedstock}}$ in kmol/h) in the feedstock [39-41].

$$\eta_c = \frac{\dot{n}_{c_{Products}}}{\dot{n}_{c_{feedstock}}} \quad \text{Equation 1}$$

ii. *Hydrogen conversion efficiency* (η_H), as determined by **Equation 2**, indicates the extent to which hydrogen entering the system's boundaries is converted into the desired fuel products. This efficiency is calculated as the ratio of the hydrogen content in the hydrocarbon product to the hydrogen content in the feedstock including that for hydrogenation [39, 42].

$$\eta_H = \frac{\dot{n}_{H_{Products}}}{\dot{n}_{H_{feedstock}}} \quad \text{Equation 2}$$

iii. *Energy ratio* (η_e): establishes the ratio between the useful energy from the products obtained (SAF, biodiesel, bio-naphtha) and the energy of the inputs used (energy per biomass), as expressed in **Equation 3**. The energy values for both the products and inputs are calculated by multiplying the material flow by the calorific value (LHV) [7].

$$\eta_e = \frac{\Sigma E_{Products}}{\Sigma E_{biomass}} \quad \text{Equation 3}$$

357 Where: $E_{products} = m_{products} * LHV_{products}$; $E_{biomass} = m_{biomass} * LHV_{biomass}$;

358 $E_{products}$ is the energy from the products obtained (MJ), $m_{products}$ is the mass of products
 359 obtained (kg), $LHV_{products}$ is the lower heating value of products (MJ/kg), $E_{biomass}$ is the energy of
 360 biomass (MJ), $m_{biomass}$ is mass of biomass (kg), $LHV_{biomass}$ is the lower heating value of biomass
 361 (MJ/kg).

362 iv. *Global plant efficiency* (η_{global}): establishes the overall energy efficiency of the process by taking
 363 into account as a ratio between (the useful energy from the products obtained and the electrical
 364 power energy produced) and energy of the biomass, as expressed in **Equation 4** [7].

$$\eta_{global} = \frac{\Sigma E_{Products} + E_{pp}}{\Sigma E_{biomass}} \quad \text{Equation 4}$$

365 Where: $E_{products}$ is energy from products (MJ); $E_{biomass}$ is energy of biomass (MJ); E_{pp} is
 366 electrical power energy produced (MJ).

367 v. *Overall energy efficiency for AtJ process*: establishes the ratio between the useful energy from
 368 the products obtained and the electrical power produced, and the energy of the biomass and
 369 electrical power energy consumed as expressed in **Equation 5** [7].

$$\eta_{AtJ} = \frac{\Sigma E_{Products} + E_{pp}}{\Sigma E_{biomass} + E_{pc}} \quad \text{Equation 5}$$

370 Where: $E_{products}$ is energy from products (MJ); $E_{biomass}$ is energy of biomass (MJ); E_{pp} is
 371 electrical power energy produced (MJ), and E_{pc} is electrical power energy consumed (MJ).

372 The second law of thermodynamics provides the basis for calculating total exergy destruction in
 373 the plant and for distributing this destruction among the individual processes or components,

highlighting the sources of irreversibility. The following performance: indicators are defined based on second law of thermodynamics.

vi. Exergetic efficiency (η_{exe}): establishes the efficiency based on the second law, as expressed in **Equation 6**, deals with the ratio between the sum of the net electric power produced by the system and the exergy of each product divided by exergy per biomass [7]:

$$\eta_{exe} = \frac{\Delta E_{PP} + \dot{B}_{SAF} + \dot{B}_{naphtha} + \dot{B}_{biodiesel}}{\Sigma \dot{B}_{biomass}} \quad \text{Equation 6}$$

Where: η_{exe} is exergetic efficiency, ΔE_{pp} is net electric power energy produced (MJ), $\dot{B}_{SAF}$ is exergy of SAF (MJ), $\dot{B}_{naphtha}$ is exergy of naphtha (MJ), $\dot{B}_{biodiesel}$ is exergy of biodiesel (MJ), $\dot{B}_{biomass}$ is exergy of biomass feedstock (MJ).

vii. Balance of exergy and exergy destroyed ($\dot{E}_d$): establishes the irreversibility and energy destruction in the system by application of heat, pressures and chemical synthesis for biomass conversion to biofuel. **Equation 7** expresses the destruction of exergy, based on a steady state, hence the balance between exergy inflows and outflows [7].

$$\Sigma \left(1 - \frac{T_0}{T}\right) Q - W + \Sigma m_{in} ex_{in} - \Sigma m_{out} ex_{out} - B_d = 0 \quad \text{Equation 7}$$

Where: $\left(1 - \frac{T_0}{T}\right) Q$ is time rate of exergy transfer accompanying heat transfer, at the rate, Q . T stands for instantaneous temperature, m_{in} is mass flow at inlet (kg), m_{out} is mass flow at outlet (kg), ex_{in} is exergy flow at inlet per unit mass (MJ/kg), ex_{out} is exergy flow at outlet per unit mass (MJ/kg), and B_d is exergy destruction (MJ).

2.5 Economic Evaluation

The techno-economic assessment evaluates the commercial viability of the integrated biorefinery on an nth-of-a-kind (NOAK) basis, representing mature commercial deployment without the cost premiums and scale-up uncertainties characteristic of first-of-a-kind (FOAK) facilities [4]. Capital expenditure (CAPEX), operating expenditure (OPEX), revenues from SAF, bio-

395 naphtha, biodiesel and surplus electricity, and the Minimum Jet Fuel Selling Price (MJSP) were
 396 determined using discounted cash flow analysis.

397 The principal economic and financing assumptions are summarised in **Table 3**. Capital-cost
 398 estimation, equipment scaling, and installation factors were adopted from Michaga et al. [39],
 399 with costs escalated to the 2024 basis using the Chemical Engineering Plant Cost Index
 400 (CEPCI)[43]. Detailed CAPEX/OPEX calculations, scaling relationships, and supporting
 401 assumptions are provided in **Supplementary Material A-1**.

Table 3. nth Plant Economic Assumptions [4, 39]

Economic parameters	Basis
Plant Design	
Base year for analysis	2024
Plant life	30 years
Optimum plant size:	2000 MT/day (DM)
Products	SAF, coproducts - biodiesel, naphtha, electricity
Location	UK (middle of wheat farmland)
Land space for infrastructure	25%
Land space for wheat cultivation	75%
Financing	
Plant financing debt/equity	60%/40% of TCI
Interest rate	9% annually
Term	10 years
Revenue	
Minimum acceptable internal rate of return	10%
Income tax rate	35%
Construction	
Construction period	3 years
Fixed capital expenditure schedule	(8% 1st year, 60% 2nd year, 32% 3rd year) ^a
Start-up	

Start-up time	6 months
Revenues during start-up	50%
Variable costs during start-up	75%
Fixed costs during start-up	100%
Operation	
On-stream availability factor	97% (8400 operating hours per year)
Plant depreciation schedule	7 years
Depreciation method	Straight line
Plant salvage value	No value
^a The percentage of the cost of the project cost throughout each year of construction.	

Detailed methodology for CAPEX and OPEX calculations is provided in **Supplementary Material A2.3**.

2.5.1 Minimum Jet Fuel Selling Price

The Minimum Jet Fuel Selling Price (MJSP) was determined using discounted cash flow analysis (DCFA) as the SAF selling price corresponding to a net present value (NPV) of zero at a minimum internal rate of return (IRR) of 10% [7, 17]. The analysis assumes an nth-plant design [14], with the principal economic assumptions summarised in **Table 3**.

Annual revenues were calculated from SAF and co-product production, as reported in **section 3.2.3, Plant Revenue**. CAPEX was distributed over the three-year construction period (8%, 60%, and 32%), with a six-month start-up period incorporated into OPEX. Straight-line depreciation over seven years, a 30-year project lifetime, and zero salvage value were assumed.

2.5.2 TEA Sensitivity and Uncertainty Analyses

Sensitivity and uncertainty analyses were conducted for the principal techno-economic parameters using the nominal, optimistic, and pessimistic values summarised in **Table 4**. APEX was varied by $\pm 30\%$, consistent with the uncertainty range associated with early-stage cost

estimates and providing a conservative basis for the NOAK scenario [44]. Fixed operating and maintenance costs (FOM) were varied by $\pm 20\%$, while feedstock costs, the principal contributor to variable operating costs (VOC), were varied by approximately $\pm 30\%$ to represent UK market volatility. The discount rate was varied by $\pm 20\%$ around the base case [28, 45], and corporate tax between 0–20% [28].

Table 4: TEA sensitivity and uncertainty analyses variables

Parameter	Basis	Low value	Nominal value	High value
Fixed Operating Cost (MM£)	$\pm 20\%$	84.5	105	126
Feedstock Cost (MM£)	$\pm 30\%$	58.33	81	108
CAPEX (MM£)	$\pm 30\%$	332	475	616
Discount rate (%)	$\pm 20\%$	8	10	12
Tax rate (%)	0-20%	0	30	36

Deterministic sensitivity was evaluated using a tornado analysis based on piecewise-linear variation of individual parameters. The Monte Carlo uncertainty analysis was conducted using uniform probability distributions for the uncertain parameters, bounded by their respective optimistic and pessimistic values. During each trial, all parameters were sampled simultaneously and independently within their specified ranges, and 100,000 trials were performed to generate the resulting MJSP probability distribution..

2.5.3 Economies of Scale

Economies of scale were evaluated over plant capacities of 1,000–4,000 t/day relative to the 2,000 t/day base case. Process-area CAPEX and OPEX were scaled according to **Equation 8**, using scaling exponents of 0.6 for CAPEX, 0.7 for fixed OPEX, and 1.0 for variable OPEX.

$$C_i(Q) = C_i(Q_0) \left(\frac{Q}{Q_0} \right)^k \quad \text{Equation 8}$$

where $C_i(Q)$ is the capital cost of the process at section i , $C_i(Q_0)$ is the reference cost at the base capacity (2,000 ton/day), k is the applicable scaling exponent.

CAPEX was annualised using a capital recovery factor based on a 10% discount rate and 30-year project life and combined with scaled OPEX to determine the annualised production cost and corresponding MJSP. The methodology was anchored to the base-case MJSP of approximately £1.40/kg at 2,000 t/day. Detailed annualization and MJSP calculations are provided in **Supplementary Material A2.3.3**.

2.6 Environmental Life Cycle Evaluation

Environmental performance with contributions at subsystem levels was evaluated using a well-to-wake (cradle-to-grave) life cycle assessment (LCA) in accordance with ISO 14040/14044 [26,79,80]. The model was implemented in SimaPro v9.6 using process-specific inventories from the Aspen Plus® simulation and background datasets from Ecoinvent to quantify life-cycle environmental impacts, including greenhouse gas emissions expressed as CO₂-equivalents.

The LCA framework comprises goal and scope definition, life cycle inventory (LCI), life cycle impact assessment (LCIA), and interpretation, as illustrated in **Figure 4** [26, 39, 46].

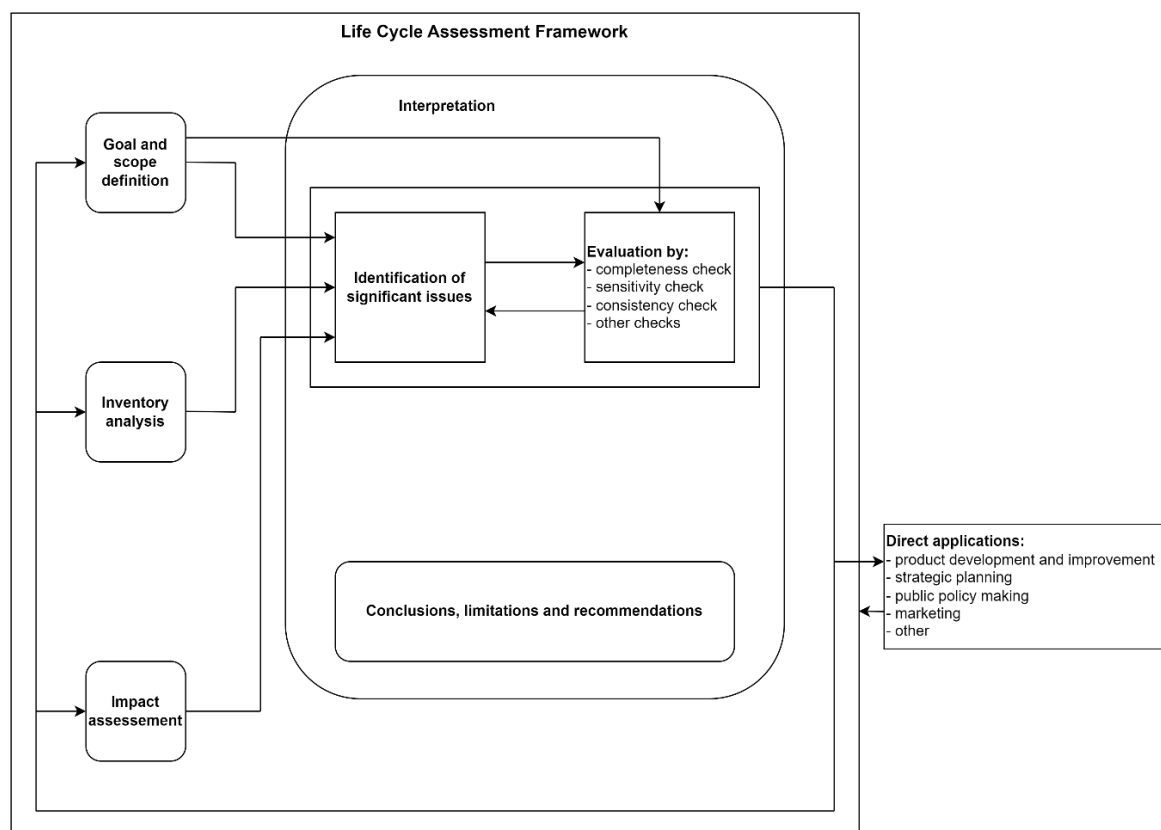


Figure 4. Life Cycle Analysis Methodology [26]

2.6.1 Goal and Scope Definition

Following ISO 14040/44, the LCA goal, functional unit, and system boundaries were defined to evaluate the life-cycle environmental performance of lignocellulosic Alcohol-to-Jet (AtJ) SAF relative to conventional Jet A-1 [47]. The functional unit was 1 MJ of jet-fuel energy delivered to the aircraft, consistent with established SAF assessment practice [28, 39, 48, 49].

A well-to-wake (cradle-to-grave) system boundary was adopted, encompassing feedstock production and collection, transportation, fuel conversion, ancillary material and energy inputs, fuel distribution, and aircraft combustion, as illustrated in **Figure 5**. This boundary is consistent with established SAF life-cycle assessments [50-53] and includes relevant upstream and downstream contributions, including chemical and energy inputs and land-use-related emissions.

Environmental performance was principally evaluated using global warming potential (GWP), expressed as g CO₂-eq/MJ, enabling comparison with conventional jet-fuel benchmarks, including the 89 g CO₂-eq/MJ fossil reference reported by Vardon et al. Fossil and non-CO₂ greenhouse gas emissions were included throughout the life cycle, [50-53], while the results of the treatment of biogenic CO₂ and land-use effects is as reported under section 3.3.1.

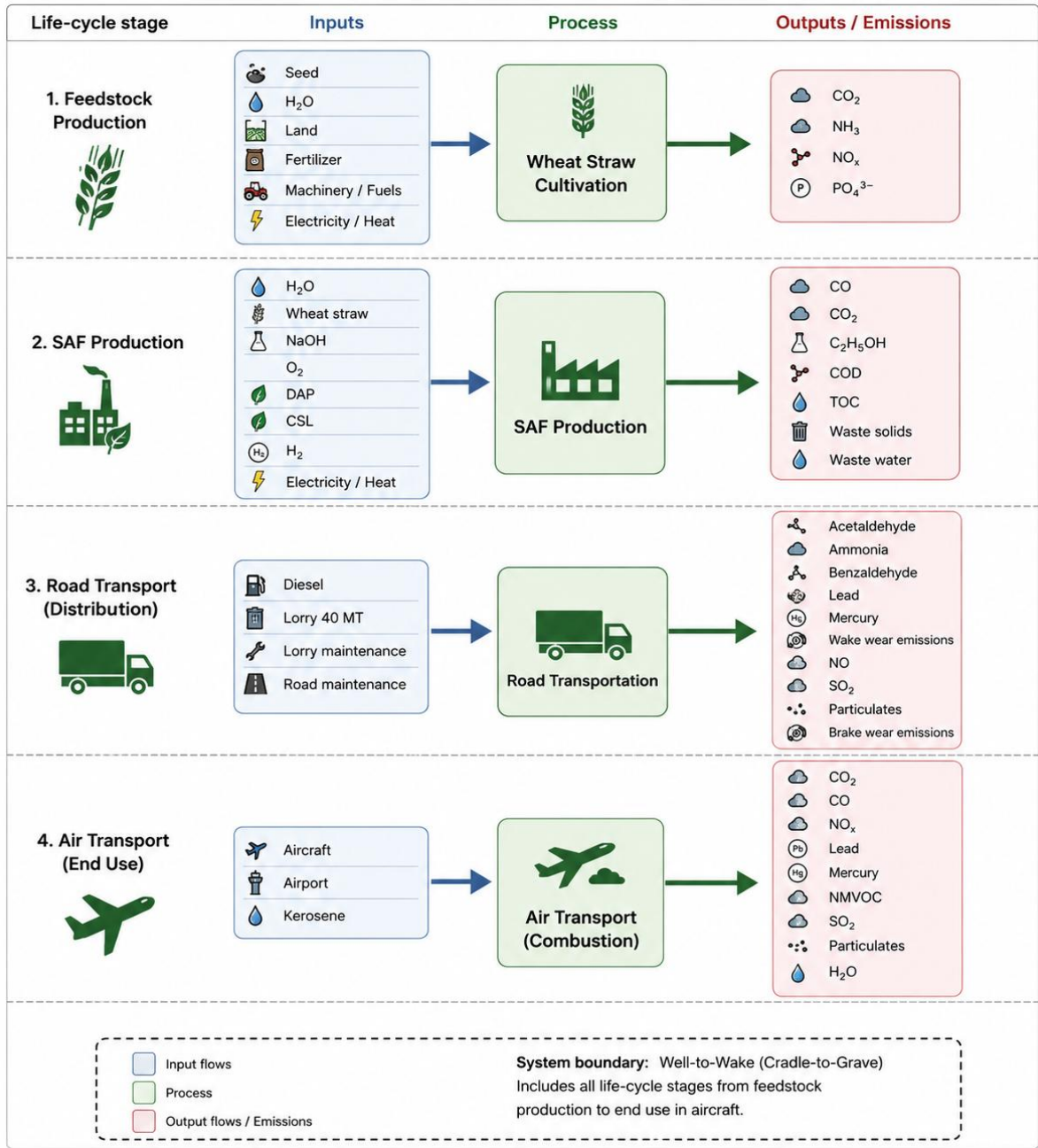


Figure 5. Environmental Life Cycle Analysis Scope

2.6.2 Allocation Procedure

Environmental burdens were distributed among SAF and energy-bearing co-products using energy-based allocation, based on their annual energy outputs calculated from product quantities and lower heating values (LHVs). The resulting allocation factors are summarised in **Table 5**.

Table 5. Energy-Based Allocation of Environmental Burdens

Allocation Factors	Quantity (x10 ⁶)	Unit	LHV (MJ/kg)	Energy conversion, MJ, (x10 ⁹)	%
Heat (useful exergy)	112.16	MJ	-	0.112	2
SAF	55.18	kg	43	2.37	43.2
Bio-naphtha	12.84	kg	43	0.55	10
Bio-diesel	12.53	kg	38	0.48	8.6
Electricity surplus	1,993.71	MJ	-	1.99	36.2
			Total	5.5	100

2.6.3 Environmental Life Cycle Inventory and Modelling

The life cycle inventory (LCI) combined foreground process data from the Aspen Plus® simulation with background datasets from Ecoinvent v3.9 and UK-specific agricultural and logistics data. The model was implemented in SimaPro 9.6.1 using ReCiPe 2016 Midpoint and IPCC 2021 GWP100 characterisation methods [54]. **Table 6** summarises the principal foreground inputs and outputs associated with SAF production.

Background modelling encompassed wheat-straw production, feedstock and fuel transportation, and aircraft end use, consistent with the well-to-wake system boundary shown in **Figure 5**. The UK case study assumes co-location of biomass pretreatment, ethanol production and AtJ upgrading, with SAF transported approximately 200 km to the end-use airport hub. Detailed

Ecoinvent process selections, regional proxies, inventory assumptions, and site-specific parameters are provided in **Supplementary Material A2.4.6**.

Table 6. SAF Production Input-Output

	Inputs	Outputs
Technosphere	NaOH (modelled at 5 wt% of dry biomass) DAP(0.33 g/L) and CSL (0.25 wt%) of fermentation broth, as per NREL technical guidelines [13]	<u>Products:</u> SAF, bio-naphtha, bio-diesel, surplus electricity, and exergy (LHV applied for the energy quantities) <u>Waste:</u> Ash and wastewater, modelled through appropriate disposal and treatment pathways.
Nature	Water drawn from freshwater sources	-
Emissions	-	Biogenic CO ₂ , CO, minor ethanol losses, and water vapour volatilisation

2.6.4 Environmental LCA Sensitivity and Uncertainty Analyses

Sensitivity analysis was performed by varying selected life-cycle inventory parameters within ± 10 -30% of their base-case values, consistent with established LCA frameworks [55, 56], and SAF assessment practices [57]. Where explicit statistical variances were unavailable, fixed uncertainty ranges were applied [58]: $\pm 20\%$ for major inventory flows, including biomass, chemicals, fertilisers and co-products, and $\pm 10\%$ for freshwater because of its comparatively low GWP contribution [59]. The parameter-specific ranges are summarised in **Table 7**.

Table 7: Deviation range for E-LCA sensitivity and uncertainty analyses

GWP Impacts	
Parameter	Deviation
Biomass feedstock	$\pm 20\%$
	$\pm 30\%$
NaOH	$\pm 20\%$
DAP	$\pm 20\%$
CSL	$\pm 20\%$
Freshwater input	$\pm 10\%$
	$\pm 20\%$

Stochastic uncertainty was evaluated using a delta-based Monte Carlo approach with independent uniform sampling within the selected low–high bounds. The resulting GWP for each trial was calculated using **Equation 9**.

$$GWP_{MC} = GWP_{base} + \sum_{i=1} \Delta_i \quad \text{Equation 9}$$

Where GWP_{MC} is the Monte Carlo Global Warming Potential, GWP_{base} is the base case value of Global Warming Potential, Δ_i is each variable parameter $\sim U(\text{low delta}, \text{high delta})$.

Alternative wider ranges ($\pm 30\%$ for biomass and $\pm 20\%$ for freshwater) were examined as sensitivity cases but excluded from the base-case Monte Carlo specification to avoid double counting. They were used as stress-test scenarios to assess the robustness of the results under greater variability.

2.7 Social Life Cycle Assessment

Social life cycle assessment (S-LCA) may be implemented using bottom-up approaches based on site-specific microeconomic data [60] or top-down approaches employing input-output models for system-wide assessment [20, 61]. Following the ISO 14040/44 framework, this study adopted a top-down approach to assess potential social risks associated with the AtJ SAF life cycle.

The assessment was implemented in SimaPro v9.6 using the Product Social Impact Life Cycle Assessment (PSILCA) database and its Social Impact Weighting Method. PSILCA employs a Multi-Regional Input-Output (MRIO) framework to link sectoral monetary flows with social-risk indicators across countries and supply chains [62]. Social risks were characterised as medium risk hours (mrh) for the principal life-cycle stages comprising wheat-straw production, SAF production in the UK, and transportation.

To the authors' knowledge, this represents the first application of PSILCA to compare social-risk contributions across multiple stages of an AtJ SAF system. Although the sector- and country-level proxy data used by PSILCA limit process-specific and sub-national representation [63-65], the approach provides a consistent basis for screening supply-chain social-risk hotspots and identifying priority areas for further assessment.

2.7.1 Objective and Scope

The S-LCA assessed potential social risks associated with wheat cultivation, SAF production, and road transport, while the aircraft-use phase was excluded because of its limited relevance to the social-risk assessment [66]. Life-cycle and plant process stages were mapped to representative PSILCA country-sector proxies for the MRIO analysis. The complete sector mappings and their functional-equivalence justifications are provided in **Supplementary Material A2.4.6**.

2.7.2 PSILCA Framework

PSILCA uses a Multi-Regional Input-Output (MRIO) framework to link monetary flows to country- and sector-specific social-risk indicators. Process-level CAPEX and OPEX flows were mapped to the corresponding PSILCA sectors and converted to labour activity using sector-specific labour-intensity coefficients. Labour hours were subsequently weighted by social-risk characterisation factors to obtain medium risk hours (mrh) [19]:

$$LH_i = M_i \times LI_i \quad \text{Equation 10}$$

$$MRH_i = LH_i \times CF_i \quad \text{Equation 11}$$

where M_i is the monetary flow (USD), LI_i is the labour intensity (h/USD), LH_i is the corresponding labour activity (h), and CF_i is the PSILCA risk characterisation factor (mrh/h). Risk levels were weighted by the CF_i as no risk = 0, very low = 0.01, low = 0.1, medium = 1, high = 10, and very high

= 100 [19]. MRH_i is the medium risk hours (mrh). Contributions were aggregated across processes and normalised to 100% for each social indicator to facilitate comparison of relative social-risk contributions as indicated in **Equation 12**.

$$C_i = \frac{MRH_i}{\sum_{j=1}^n MRH_j} \times 100 \quad \text{Equation 12}$$

where C_i is the normalised contribution of process to a given social indicator.

2.7.3 Process Mapping and Data Allocation

Process stages were mapped to representative PSILCA country-sector proxies, with the detailed mappings and functional-equivalence justifications provided in **Supplementary Material A2.4.6**. Life-cycle economic flows were derived over the 30-year operating period and converted to USD for PSILCA modelling. These flows were normalised to the functional basis used for the S-LCA, yielding 0.023 kg/MJ for SAF and co-products, £0.015/MJ for biomass, and £0.036/MJ for transport, which were used to determine cost-linked social-risk intensities across foreground and background processes.

2.7.4 Geospatial Distribution Modelling

PSILCA sector-level social-risk results were aggregated by ISO3 country code in Excel to obtain country-level medium risk hours (mrh). The aggregated results were subsequently linked to a global shapefile in QGIS to visualise the geographical distribution of social-risk hotspots.

3 Results and Discussion

The thermodynamic, economic, environmental and social assessment performances are provided in the subsequent subsections.

3.1 Thermodynamics Performance

Table 8 summarises the annual mass and energy balances of the integrated biorefinery. At approximately 0.7 MMT/year wheat-straw throughput, the plant produces 52,912 t/year SAF and 24,343 t/year of bio-naphtha and biodiesel co-products. Internal utility integration satisfies process demands while enabling approximately 48 MW (1.45 PJ/year) of net electricity export, with the electrolyser meeting the 244 kg/h hydrogenation requirement. Surplus hydrogen, oxygen, nitrogen and other industrial gases provide additional opportunities for co-product valorisation.

3.1.1 Mass Balance and Conversions

Mass and atomic balances showed negligible inlet–outlet discrepancies, confirming mass conservation across the simulated process. As summarised in **Table 8**, approximately 22% of feedstock carbon was converted to fuel products, with 15% converted to SAF; product carbon selectivity was 69% SAF, 15% bio-naphtha and 16% biodiesel. Similarly, 27% of feedstock hydrogen was recovered in fuel products, comprising 19% in SAF and 8% in the other fuel products, with product hydrogen selectivity of 70%, 15% and 15%, respectively.

On a mass basis, SAF and total fuel-product yields were approximately 8% and 11% of dry biomass, respectively, corresponding to a SAF mass selectivity of 68%. Detailed mass and atomic balances are provided in **Supplementary Material A5.0** while detailed consumable requirements are considered in **Section 3.2.2.1, Variable Operating Cost**.

Table 8: Plant Throughput-Output

Components	Quantity	Unit
Main Process Plant		
Inputs		
Wheat Straw (Biomass)	83,333	Kg/hr
Water	2,070	m ³ /hr
Oxygen	4.11	Kg/hr
NaOH	4.11	Kg/hr
Hydrogen	244	Kg/hr
Outputs		
SAF	6,299	Kg/hr
Bio-naphtha	1,465	Kg/hr
Bio-diesel	1,433	Kg/hr
Electricity surplus	48.18	MW
Exergy (useful energy)	3.56	MW
Electrolyzer		
Excess hydrogen	36.87	Kg/hr
Oxygen produced	140.41	Kg/hr
Air Separation Unit		
O ₂ liquid	734.02	Kg/hr
N ₂ gas	4,086.76	Kg/hr
N ₂ liquid	398.40	Kg/hr
Argon	73.89	Kg/hr

585 3.2 Economics Performance

586 The economic performance is evaluated in terms of capital and operating expenditures,

587 plant revenues, sensitivity and uncertainty, and economies of scale.

3.2.1 CAPEX

The total capital investment was estimated at approximately £475 million, comprising a PEC of £176 million and IDC of £307 million. The IDC is broadly comparable in magnitude with previous techno-economic assessments of lignocellulosic biorefineries at approximately 2,000 t/day capacity, including Humbird et al. [13], Kazi et al [14] and Yuan et al. [67]. and Mohsenzadeh [38], as detailed in **Supplementary Material, A3.1**.

As shown in **Figure 6**, hydrolysis and fermentation constitute the largest capital component, £152 million, reflecting the integrated enzyme-production and recycling configuration. This exceeds the corresponding costs reported by Humbird et al. [13] and Kazi et al. [14], which exclude integrated enzyme production from their base installed costs, but is more comparable with the recent assessment of Yuan et al. [67]. Additional capital intensity arises from the integration of on-site hydrogen and oxygen production, while the £70 million lignin-fired cogeneration system supports process energy self-sufficiency and approximately 48 MW net electricity export.

Wastewater treatment [68-70], the alkaline electrolyser [71] and ASU [72] were estimated at approximately £8.8 million, £9.6 million and £25 million, respectively, using literature-derived cost bases adjusted to the required plant capacities and 2024 cost basis.

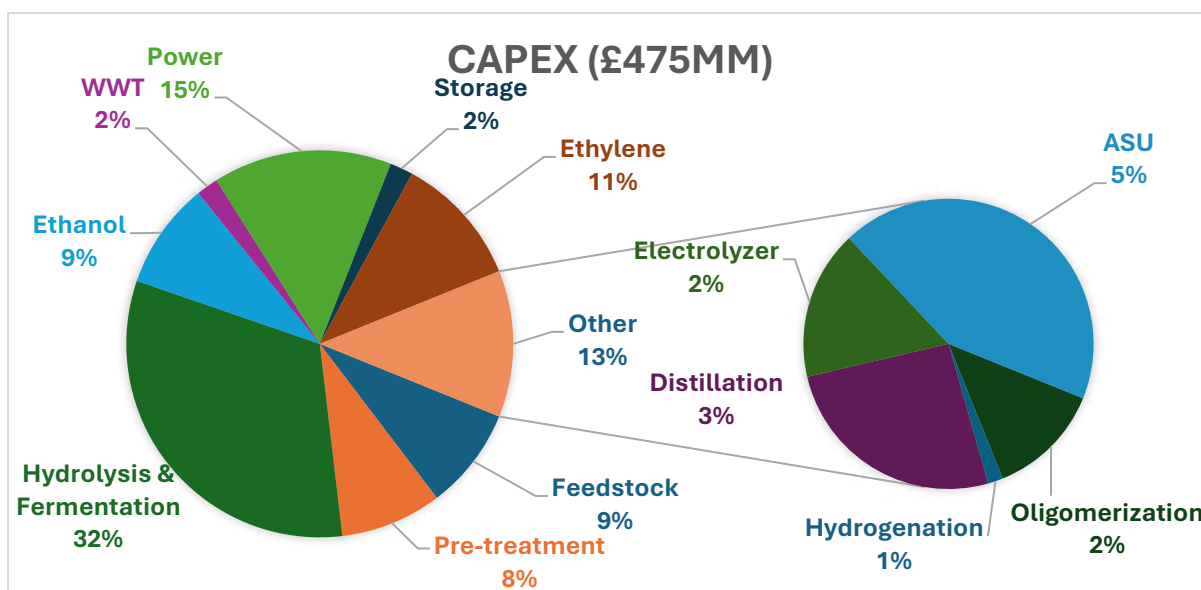


Figure 6. Capital Expenditure share by process stages.

3.2.2 OPEX

Total annual OPEX was approximately £193 million. As shown in **Figure 7**, feedstock procurement and its handling is the dominant contributor at 34%, including approximately £60 million/year in feedstock purchase costs (part of VOC), and was consequently included at $\pm 30\%$ in the economic sensitivity analysis. Hydrolysis and fermentation represent the second-largest process-area expenditure at ~£26 million/year, reflecting enzyme, nutrient and utility requirements, while hydrogenation contributes the lowest at ~£9.9 million/year. Within VOC, pretreatment and hydrolysis/fermentation account for approximately £6.9 million/year and £8 million/year, respectively. Detailed consumable quantities, catalyst replacement assumptions and unit-cost calculations are provided in **Supplementary Material A-1**.

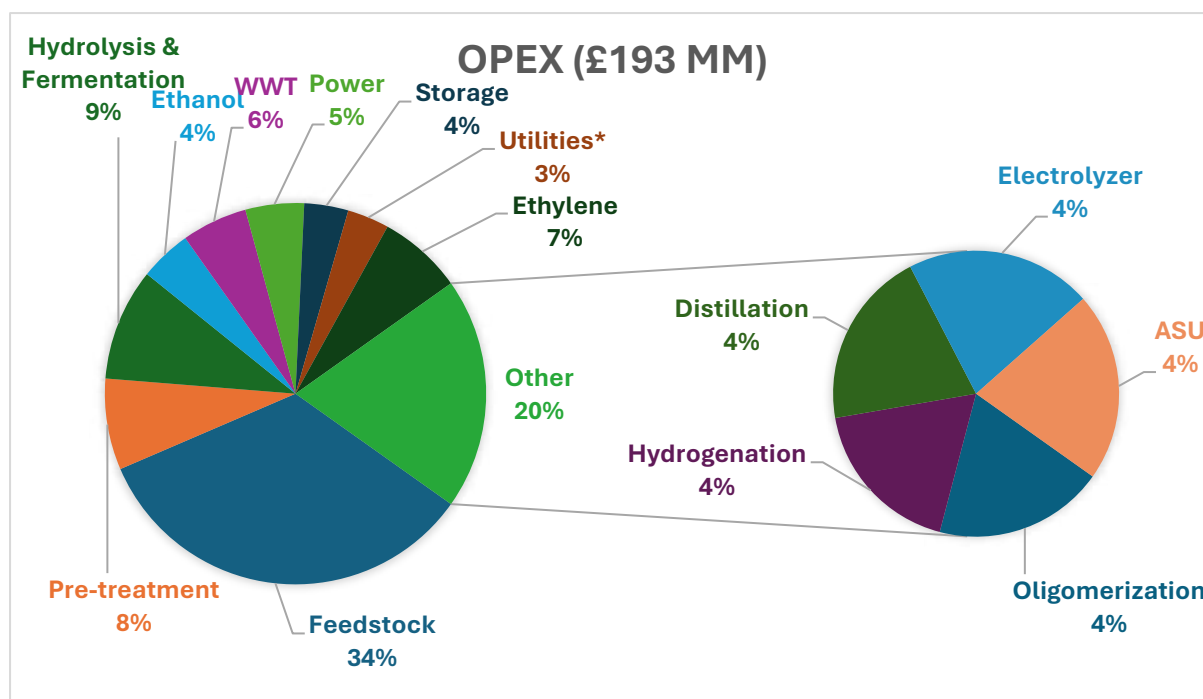


Figure 7. Operating Expenditure share by process stages

3.2.3 Plant Revenue

Co-product valorisation generates approximately £140 million/year, equivalent to ~73% of the £193 million annual OPEX and therefore provides an important offset to the Minimum Jet Fuel Selling Price (MJSP). Bio-naphtha and biodiesel contribute approximately £17 million/year and £13.3 million/year, respectively, based on market prices of approximately £740/t [73] and £1,145/t [74].

As shown in **Figure 8**, surplus electricity is the dominant revenue source, contributing approximately £103 million/year (74%), based on an a 5-year average UK electricity price of £248.6/MWh [75]. This highlights the economic importance of integrating lignin-fired cogeneration with SAF production. Hydrogen and industrial-gas co-products provide comparatively minor contributions to total revenue.

Co-Products Revenue (140 MM£)

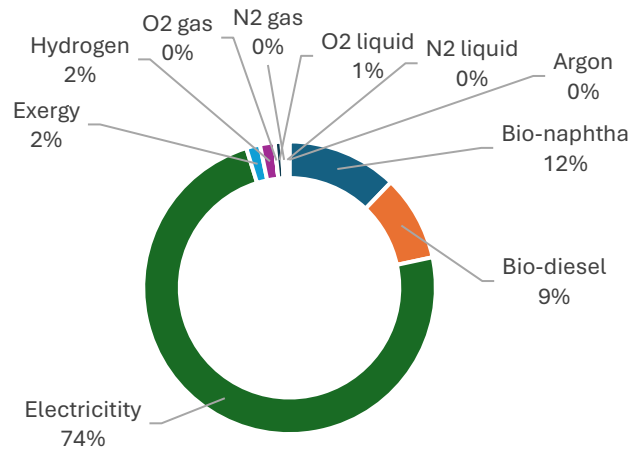


Figure 8. Annual Revenue by co-products

3.2.4 Minimum Jet Fuel Selling Price and Financing Sensitivity

The discounted cash flow analysis, based on £475 million CAPEX and £193 million/year OPEX, gives a base-case Minimum Jet Fuel Selling Price (MJSP) of approximately £1.41/kg at 40% equity financing. As summarised in **Table 9**, excluding co-product revenues, MJSP ranges from £3.53 to £4.74/kg across the financing scenarios. The co-product revenue assumptions produce MJSP values ranging from £0.78 to £2.40/kg, demonstrating the strong influence of capital structure and co-product valorisation on economic viability. The smaller MJSP observed when co-products are considered, highlights the importance of integrated revenue generation and financing strategy in determining the competitiveness of SAF production.

Table 9. Minimum Jet Fuel Selling Price per scenario.

Scenario	MJSP (£/kg)	
	with Co-products	w/o Co-products
100% Equity	0.78	3.53
40% Equity - Principal + Interest after 3 yrs	1.41	4.15
40% Equity - Principal 1st 3 yrs + Interest thereafter	2.40	4.74
0% Equity - Principal 1st 3 yrs + no Interest	2.05	4.53

3.2.5 TEA Sensitivity and Uncertainty Analyses

As shown in **Figure 9**, feedstock cost has the strongest influence on MJSP, varying the base value of £1.41/kg to approximately £1.26–1.59/kg, followed by CAPEX and fixed operating cost. In contrast, variations in tax and discount rates have comparatively limited effects. The results therefore identify feedstock procurement, capital investment and operating-cost control as the principal opportunities for improving economic competitiveness.

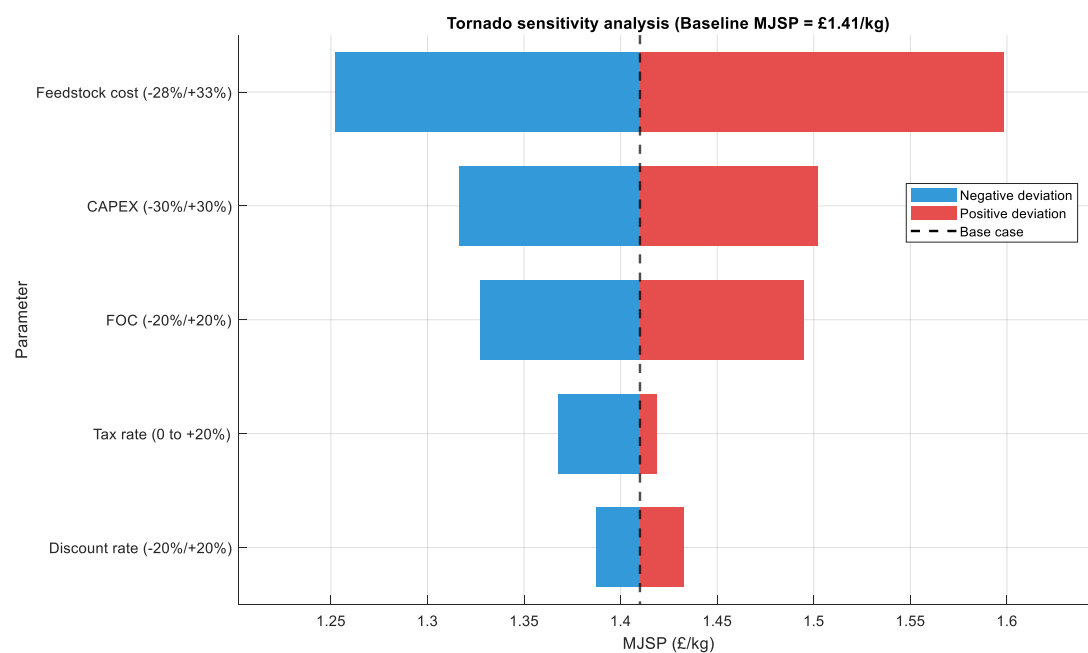


Figure 9. MJSP Sensitivity Tornado Plot

The Monte Carlo analysis, **Figure 10**, shows a broad MJSP distribution with a mean of approximately £1.0/kg and a P5–P95 range of approximately £0.50–1.45/kg. The mean lies below the deterministic £1.41/kg base case because the specified parameter ranges are collectively asymmetric around the base case, particularly for influential variables. Overall, the analyses identify feedstock, capital and operating costs as the principal sources of economic uncertainty and therefore the primary targets for cost reduction.

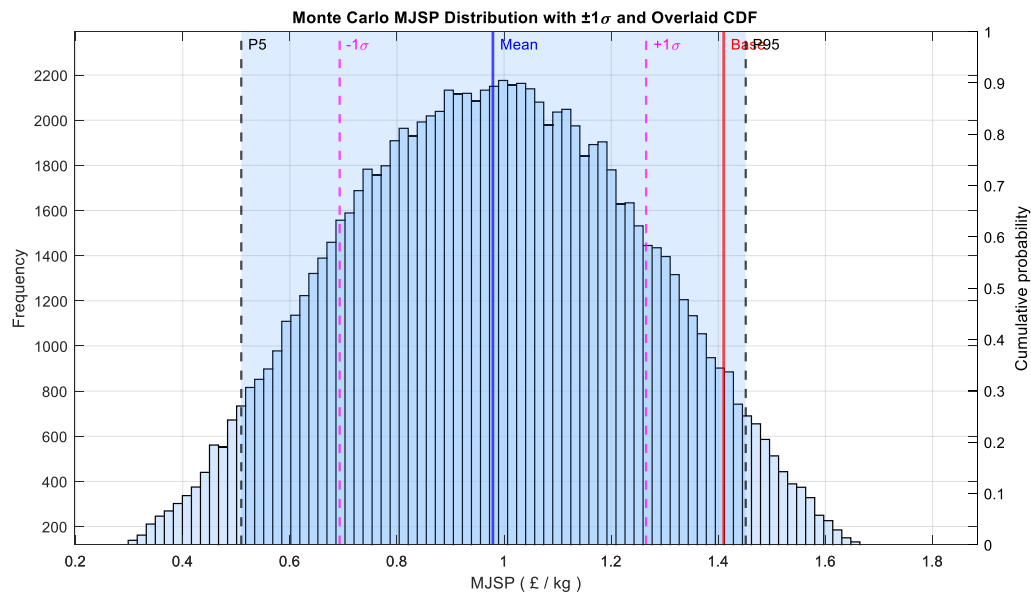


Figure 10. MJSP Monte Carlo Uncertainty Plot

3.2.6 Economies of Scale

As shown in **Figure 11**, increasing plant capacity from 1,000 to 4,000 t/day reduces the MJSP from approximately £1.61 to £1.22/kg, relative to £1.40/kg at the 2,000 t/day base case. The diminishing slope at higher capacities indicates progressively smaller gains from capital and fixed-cost dilution.

However, these theoretical scale benefits are constrained by UK feedstock availability and logistics, with realistically recoverable cereal straw estimated at approximately 2-5 Mt/year [34]. Larger facilities require wider collection radii, potentially increasing transport costs and associated environmental impacts. Consequently, practical plant sizing should balance economies of scale against regional feedstock availability and supply-chain requirements rather than pursuing maximum capacity alone.

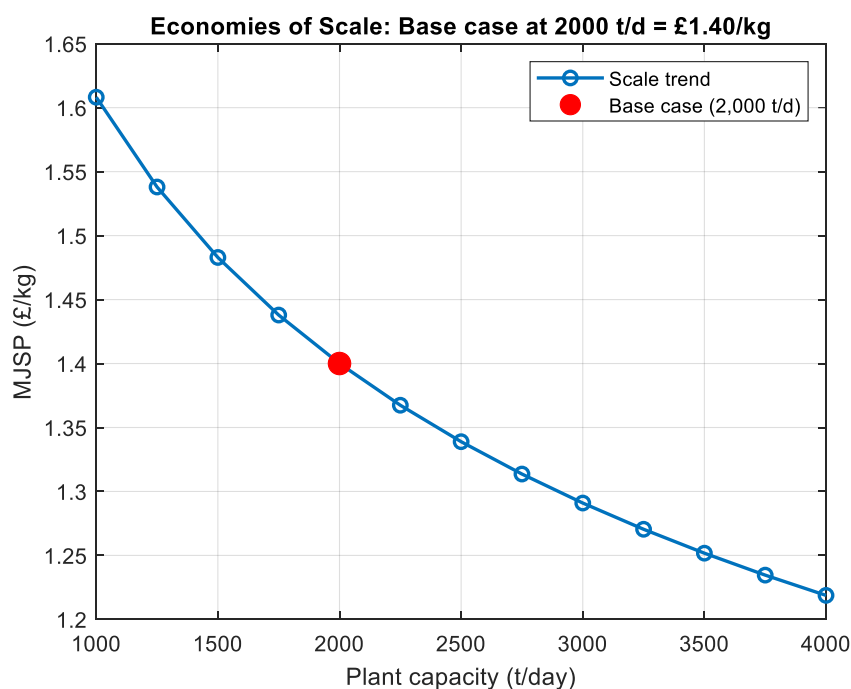


Figure 11. Effect of plant capacity on the minimum jet fuel selling price

3.3 Environmental Life Cycle Performance

The life-cycle GHG results are presented in **Figure 12** and **Figure 13** at the process-input and life-cycle-stage levels, respectively. Within SAF production (**Figure 12**), biomass feedstock is the largest individual contributor, accounting for more than half of the foreground GWP, followed principally by NaOH. These hotspots indicate that feedstock-related burdens and pretreatment chemical requirements are key targets for reducing production-stage emissions.

At the full life-cycle level (Figure 13), SAF production dominates GWP at approximately 13 g CO₂-eq/MJ, followed by transportation and logistics (~2.5 g CO₂-eq/MJ) and wheat-straw supply (~1 g CO₂-eq/MJ), while aircraft end-use contributes only 0.083 g CO₂-eq/MJ under the adopted biogenic-carbon accounting approach. The resulting total is approximately 17 g CO₂-eq/MJ SAF. The dominance of the conversion stage is consistent with the relative importance of production reported for biomass-derived aviation fuels by Pierobon et al. [48] and highlights process integration, chemical consumption and low-carbon energy supply as principal opportunities for

further GHG reduction. Indirect land-use and displacement effects are examined separately in
Section 3.3.1.

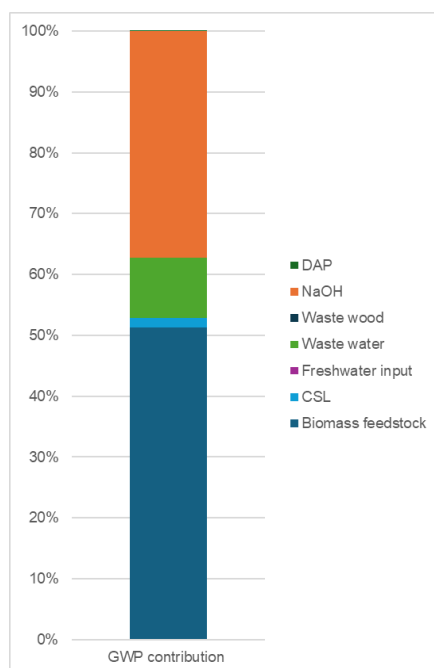


Figure 12. Contribution of process inputs to SAF production-stage GWP (Total: 13 g CO₂-eq/MJ)

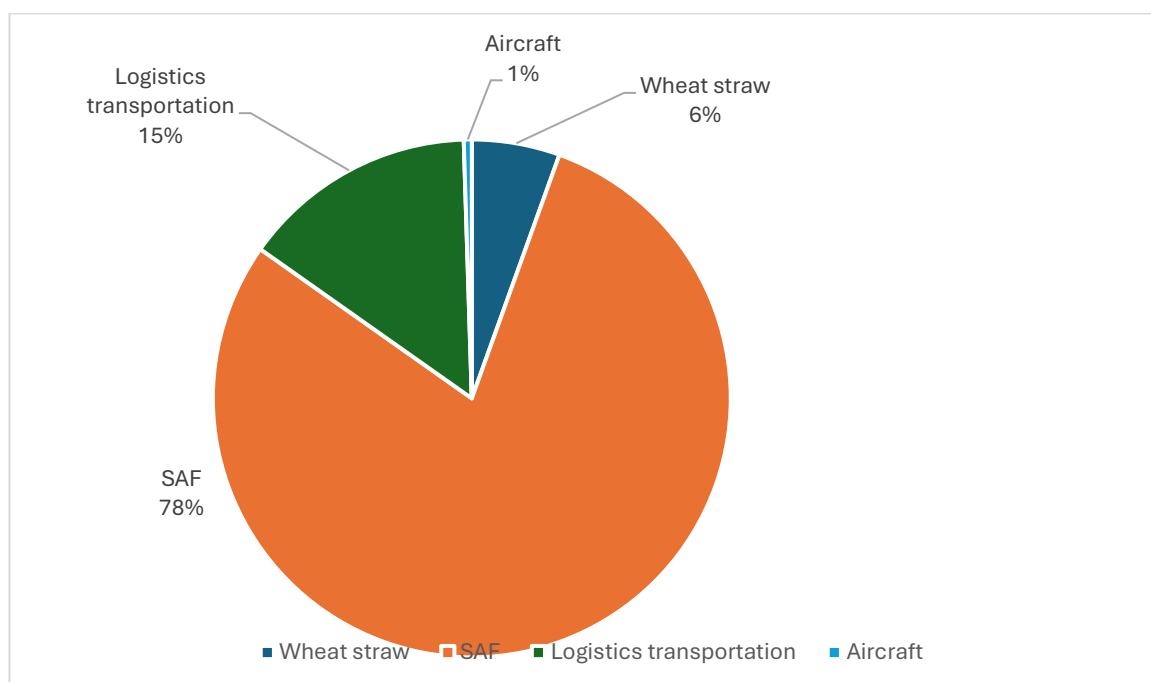


Figure 13. Contribution of life-cycle stages to well-to-wake GWP (Total: 17 g CO₂-eq/MJ)

3.3.1 E-LCA Sensitivity and Uncertainty Analyses

The sensitivity results on **Figure 14**, identify biomass feedstock as the dominant GWP driver, followed by NaOH, whereas CSL, DAP and freshwater exert substantially smaller effects. Across the tested ranges on **Table 12**, these results indicate that feedstock-related burdens and pretreatment chemical consumption are the principal targets for reducing production-stage GWP.

Table 12: Data for MJSP sensitivity and uncertainty analyses

GWP Impacts				
Parameter	Deviation	Low value (g CO ₂ eq /MJ SAF)	Nominal (g CO ₂ eq /MJ SAF)	High value (g CO ₂ eq /MJ SAF)
Biomass feedstock	±20%	11.931	13.297	14.663
	±30 %	10.519	13.297	14.351
NaOH	±20 %	11.509	13.297	13.362
DAP	±20 %	12.435	13.297	12.436
CSL	±20 %	12.395	13.297	12.476
Freshwater input	±10 %	12.436	13.297	12.436
	±20 %	12.436	13.297	12.436

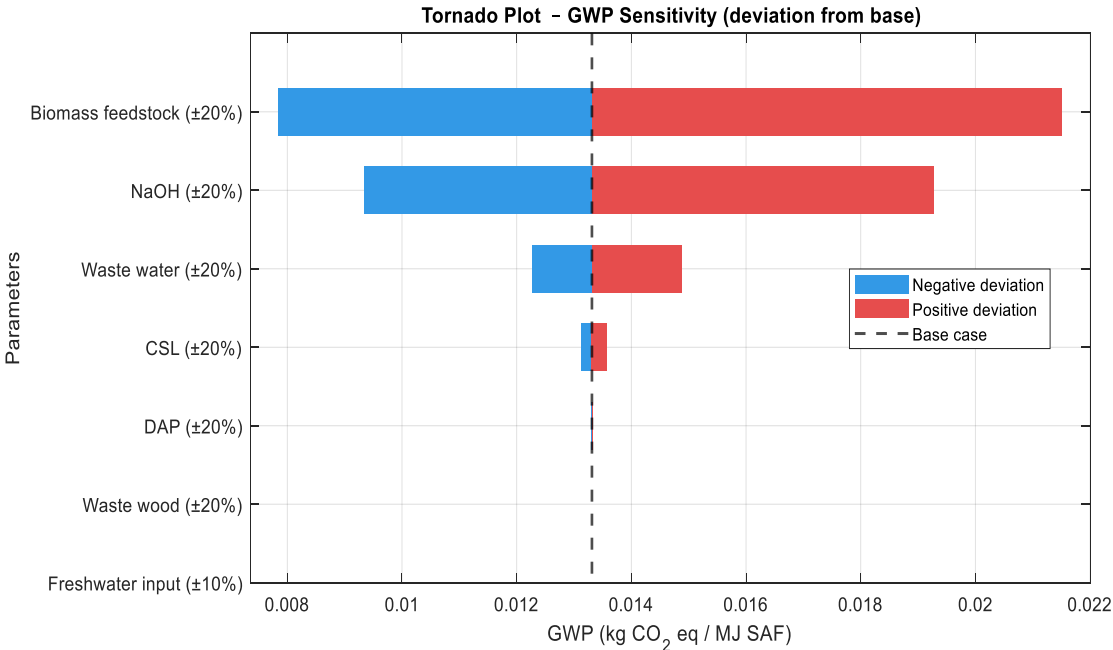


Figure 14: GWP Sensitivity Tornado Plot

The Monte Carlo analysis depicted in **Figure 15**, yields a mean production-stage GWP of approximately 16 g CO₂-eq/MJ SAF, compared with the deterministic base case of 13.3 g CO₂-eq/MJ SAF, with a P5–P95 interval of approximately 8–24 g CO₂-eq/MJ SAF. The broad uncertainty range reflects the combined propagation of variability in the selected inventory parameters and reinforces the dominant influence of biomass feedstock and NaOH assumptions. Nevertheless, even the upper percentile of SAF production-stage GWP remains substantially below the fossil-jet GHG benchmark, supporting the potential climate benefit of the pathway while highlighting the importance of robust feedstock and chemical-inventory assumptions.

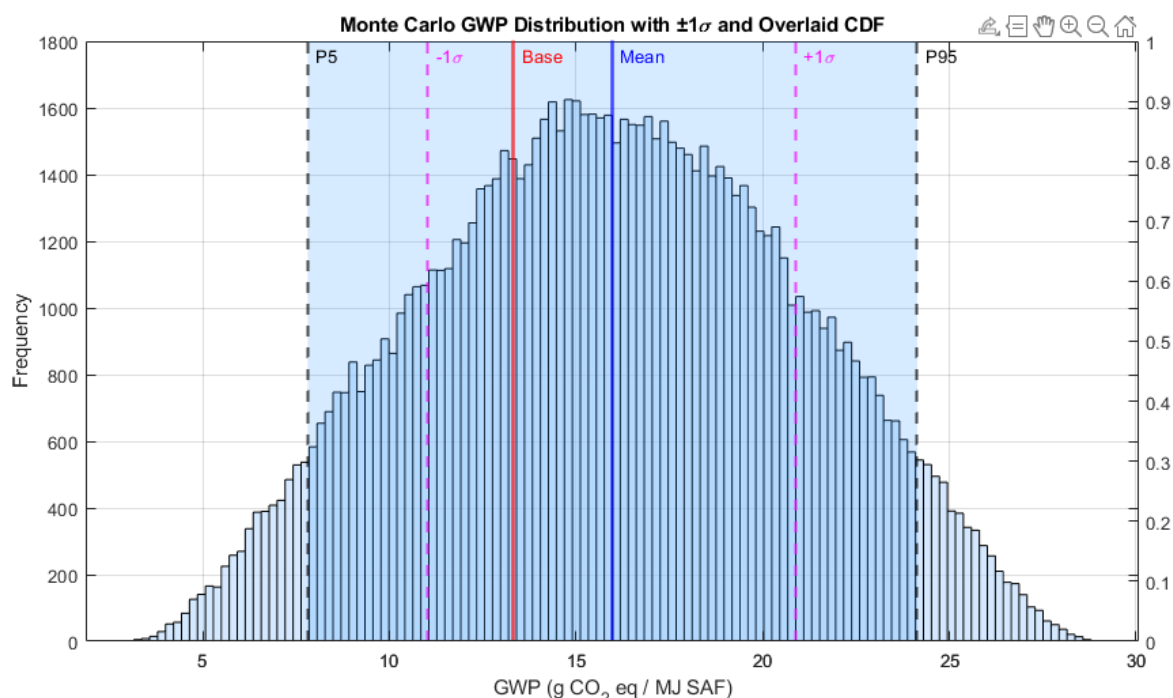


Figure 15: GWP Monte Carlo Uncertainty Plot

Impact of Indirect Land Use Change and Soil Organic Carbon accounting

Under the IPCC 2021 GWP100 method implemented in SimaPro, biogenic CO₂ uptake and emissions are excluded from impact characterisation; consequently, the reported end-use combustion impact reflects primarily non-CO₂ GHG emissions (CH₄ and N₂O). Under UK RTFO accounting, wheat straw is classified as an agricultural residue and is therefore not subject to

mandatory ILUC factors. Nevertheless, potential market-mediated displacement and soil organic carbon (SOC) effects were evaluated through sensitivity analyses.

Diversion of wheat straw from existing uses, including animal bedding and biogas production, increases GWP by approximately 2 – 3 g CO₂eq/MJ SAF through substitution-related upstream emissions. Potential SOC losses associated with residue removal were evaluated over 0.1 – 0.8 t CO₂eq/ha·yr, corresponding to approximately 3 – 22 g CO₂eq/MJ SAF, compared with literature values of approximately 8.8 – 14.9 g CO₂eq/MJ for residue-based systems. Under the high-SOC-loss scenario, total life-cycle GWP increases from approximately 17 to 39 g CO₂eq/MJ SAF. Although this substantially narrows the climate benefit, it remains more than 55% below the fossil-jet benchmark, demonstrating the importance of sustainable residue-removal practices in determining the pathway's realised GHG performance.

3.4 Social Life Cycle Performance

Of the 189 PSILCA indicators, five were selected for their relevance to the UK SAF system: fair salary, safety measures, health expenditure, education expenditure, and social security expenditure.

3.4.1 Social Risk Comparison by Phase

As shown in **Figure 16**, road transport exhibits the highest aggregated social risk, $\sim 55 \times 10^{-3}$ mrh/MJ SAF, followed by SAF and co-product production, $\sim 46 \times 10^{-3}$ mrh/MJ SAF and wheat cultivation, $\sim 29 \times 10^{-3}$ mrh/MJ SAF. Across all three phases, fair salary is the dominant indicator, while health and social-security expenditures make smaller contributions and safety and education risks remain comparatively low. The results therefore identify labour conditions, particularly within transport and industrial supply chains, as the principal social-risk hotspot.

These results should be interpreted as potential sector-level social risks rather than site-specific impacts, because PSILCA relies on macro-sector and country-level proxy data that may not capture process-specific or sub-national conditions.

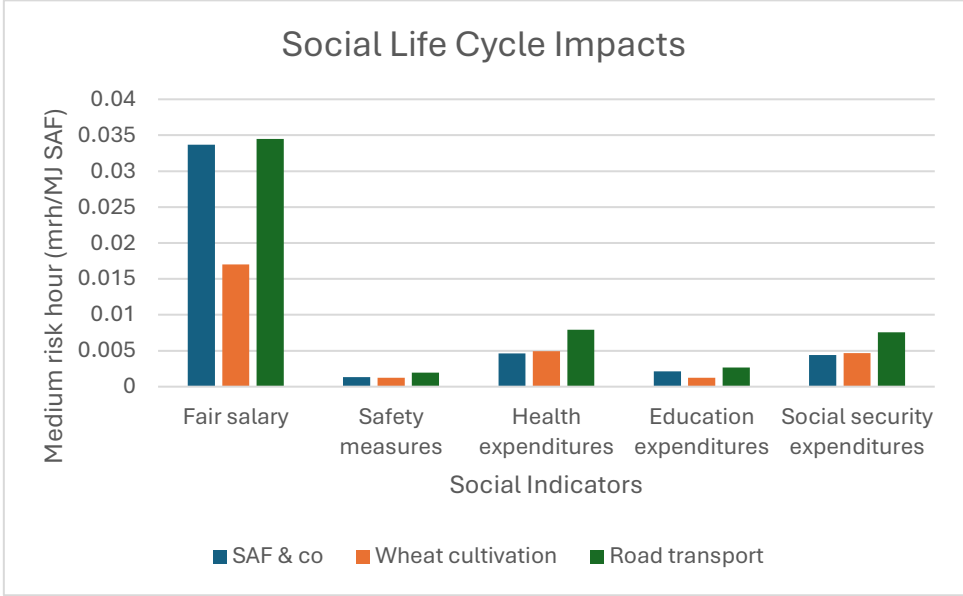


Figure 16. Social Impacts for Indicators

These results should be interpreted as potential sector-level social risks rather than site-specific impacts, because PSILCA relies on macro-sector and country-level proxy data that may not capture process-specific or sub-national conditions [76]. Nevertheless, the prominence of fair-salary risk is consistent with broader social-risk assessments highlighting wage disparities across supply chains [77]. For product-specific attribution, 68.5% of the SAF and co-product production risk is allocated to SAF according to the adopted allocation procedure.

3.4.2 Social Risk Comparison for SAF & co Products Phase

Figure 17 and **Figure 18** show the normalised process contributions to social risk for the SAF and co-products production phase, across all social indicators and the five selected indicators, respectively. *Industries – Collection, purification and distribution of water – GBR* is consistently the largest contributor, including for Health Expenditure, Fair Salary, Safety Measures, Education Expenditure, and Social Security Expenditure, indicating a cross-cutting social-risk burden

associated with water utility services. Other important contributors include *Industries – Production of ethyl alcohol from fermented materials – GBR*, *Industries – Manufacture of other general-purpose machinery – USA*, and *Industries – Fluid power machinery – USA*.

The detailed contributions of the five indicators, disaggregated by substance-risk level and process, are provided in **Supplementary Material A3.2**. Here, “substance” represents the distribution of risks from very low to very high categories, whereas “process” represents contributions from foreground and background supply-chain activities across countries.

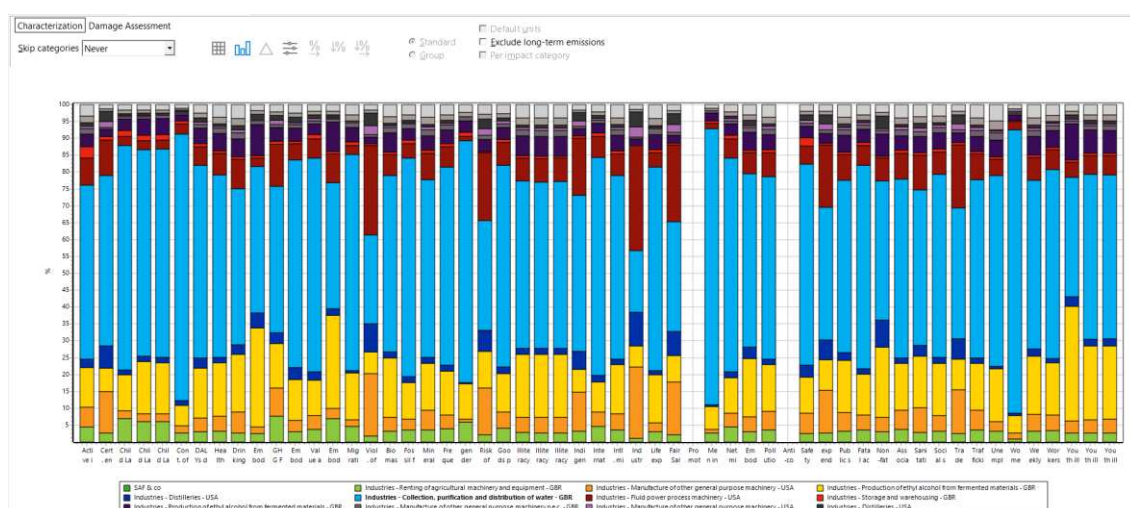


Figure 17. Foreground Process: Overall normalised contribution by process across social indicators

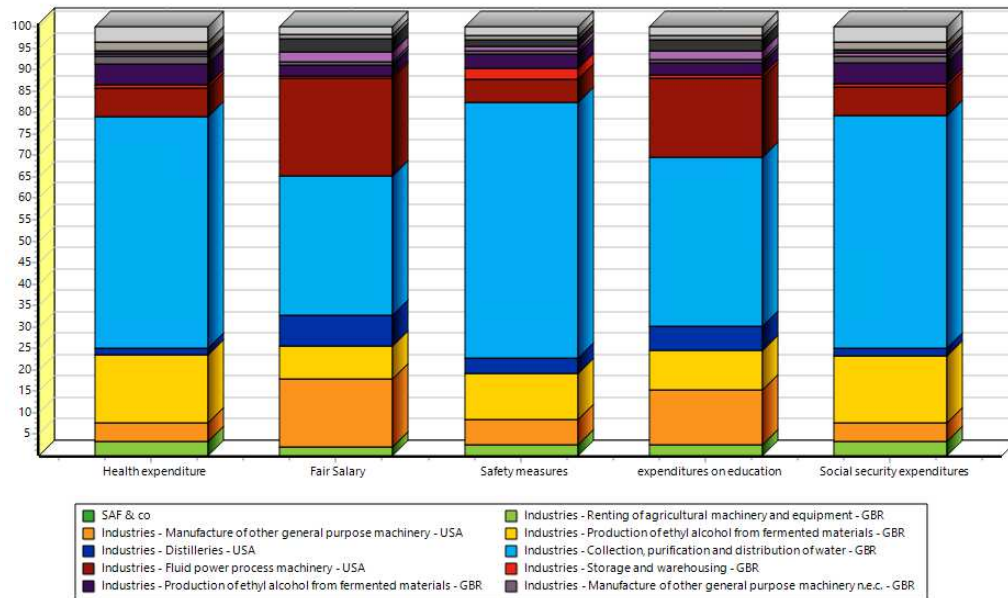


Figure 18. Foreground Process: Normalised Industry contributions across 5 selected social indicators

The geographic analysis, **Figure 19** shows that medium-risk hours are prominent across the supply chain, partly reflecting the proxy sectors and country-specific datasets used in the social-risk model. Geographic hotspots are also evident: the United Kingdom, United States, Brazil, Germany, Russia, China, and South Africa are major contributors to the Fair Salary indicator, with similar regional concentration observed for the other four indicators (safety measures, education, health, social security expenses) whose geographic risk distribution are shown in **Supplementary Material A3.11**. These results demonstrate that the social-risk profile is shaped not only by the SAF foreground process but also by geographically dispersed upstream supply-chain activities.

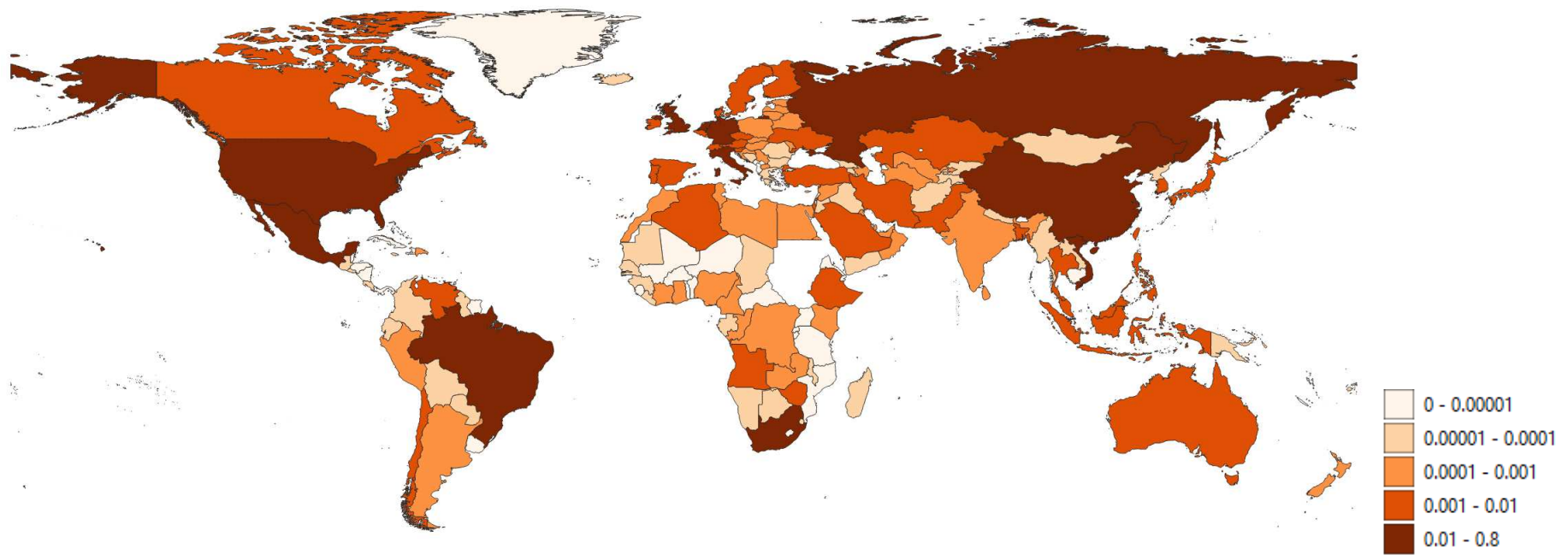


Figure 19. Geographic distribution of SAF process contributions to Fair Salary risks

3.5 UK SAF Policy and Research Implications

The UK SAF policy framework supports the scale-up of low-carbon aviation fuels, with the SAF mandate taking effect from 2025 and increasing progressively towards 10% of total UK jet fuel demand by 2030 [78]. Alongside the Renewable Transport Fuel Obligation (RTFO), this framework promotes advanced SAF pathways based on waste and residue feedstocks, including lignocellulosic materials such as wheat straw, consistent with efforts to minimise indirect land-use change and lifecycle GHG emissions [78].

The present study demonstrates the relevance of wheat-straw-derived Alcohol-to-Jet (AtJ) SAF to these objectives. As per UK SAF Mandate, the estimated supply-chain lifecycle GHG intensity of 17 g CO₂-eq/MJ SAF corresponds to a GHG reduction exceeding 80% relative to the fossil-fuel comparator (89 g CO₂-eq/MJ SAF) used in this study. The techno-economic analysis further indicates the potential for a competitive Minimum Jet Selling Price (MJSP), particularly under scenarios incorporating carbon pricing and supportive policy incentives, providing evidence relevant to future SAF price benchmarking and credit valuation.

Beyond GHG performance and cost, the environmental and social life-cycle assessments identify broader sustainability considerations relevant to SAF deployment. In particular, the S-LCA highlights supply-chain risks associated with fair salary, safety measures, health expenditure, education expenditure, and social security expenditure, demonstrating the importance of considering social as well as environmental performance when scaling SAF supply chains. Collectively, the integrated process modelling, techno-economic, environmental and social assessments provide an evidence base for evaluating lignocellulosic AtJ deployment within the UK and support the wider policy objective of achieving net-zero aviation by 2050.

3.6 Study Limitations

Despite the integrated systems modelling adopted in this study, limitations remain across the technical, economic, environmental, and social assessments.

Although the Aspen Plus® model employed validated thermodynamic and kinetic data for HZSM-5-catalysed ethanol dehydration, oligomerisation, and hydrogenation, industrial-scale performance may differ due to catalyst deactivation through coking, fouling and hydrothermal damage; heat- and mass-transfer limitations; and scale-dependent hydrodynamic effects that can affect conversion and selectivity but are not fully represented by steady-state simulations [79-82]. Predictive robustness is further constrained by limited pilot-scale data, particularly for the downstream thermochemical upgrading stages, and by variations in feedstock properties, including moisture content and lignin-to-cellulose ratio, which influence energy demand, conversion yield, and process stability [79, 83]. Furthermore, UK wheat-straw availability (~2–5 Mt yr⁻¹) and associated collection and transport requirements may constrain practical scale-up despite potential technical and economic economies of scale.

The techno-economic assessment relies partly on scaled CAPEX and OPEX data from literature and vendor information and therefore does not fully capture location-specific labour costs, inflation, infrastructure, plant scope, and contingency requirements. Operating costs also assume relatively stable prices for enzymes, hydrogen, and lignocellulosic feedstocks, although these are exposed to market and policy fluctuations [84]. Consequently, the minimum jet selling price (MJSP) remains sensitive to financial assumptions, including the 10% discount rate, 30-year plant life, and future co-product market values.

Environmental limitations arise primarily from Life Cycle Assessment (LCA) assumptions and data availability. Although the assessment followed ISO 14040/44 [26], adopted a cradle-to-grave

system boundary, and used 1 MJ SAF as the functional unit, indirect land-use change (ILUC) was excluded because of methodological uncertainty and the lack of reliable regional baselines [85-87]. For wheat straw, a residue feedstock, the more relevant uncertainty may arise from market-mediated displacement of alternative straw uses and associated soil-organic-carbon effects, rather than direct land conversion. Background inventories for chemicals, utilities, and catalysts were based partly on global-average Ecoinvent datasets and may therefore differ from UK- or site-specific conditions [88]. Uncertainties associated with fertiliser use and agricultural machinery further affect upstream emissions [89, 90]. In addition, the use of economic allocation between SAF and co-products influences the reported environmental burdens, which could differ under alternative allocation approaches such as energy-based allocation [26, 91].

The social Life Cycle Assessment (S-LCA), based on PSILCA, provides a screening-level assessment of supply-chain social risks but is constrained by national-level input-output data and proxy indicators. Its spatial and organisational resolution therefore limits assessment of site-specific issues such as land-tenure rights, labour exploitation, and gender equity [19, 20, 61]. Indicators such as fair salary and access to social security may also incompletely represent informal labour conditions, particularly in rural feedstock-producing regions [19, 20]. Furthermore, stakeholder engagement and local community feedback were not incorporated, limiting the contextual depth of the assessment [92]. Thus, while PSILCA is useful for identifying potential social hotspots, the results should be interpreted considering the uncertainties inherent in aggregated sectoral and macroeconomic data [20].

Future research should prioritise pilot-scale validation, location-specific cost and inventory data, improved treatment of ILUC and market-mediated feedstock displacement, and participatory S-LCA involving affected stakeholders. Greater spatial and process-level resolution, combined with multi-objective sustainability optimisation, would strengthen assessment of the trade-offs

between economic viability, climate mitigation, and just-transition outcomes. Emerging social-licence models [93] and context-aware S-LCA approaches [94] underscore the value of these spatially and socially grounded methods.

4. Conclusion

The aviation sector, responsible for over 2% of global CO₂ emissions, faces increasing pressure from international and national decarbonisation frameworks to accelerate the transition towards low-carbon fuels. In this context, this study comprehensively evaluated the sustainability performance of Sustainable Aviation Fuel (SAF) production via the Alcohol-to-Jet (AtJ) pathway using lignocellulosic wheat straw, integrating technological feasibility, economic viability, environmental performance, and social sustainability within a unified assessment framework.

The study combined Aspen Plus® process modelling, discounted cash-flow analysis (DCFA), ISO 14040/44-aligned Life Cycle Assessment (LCA), and PSILCA-based Social Life Cycle Assessment (S-LCA). Technically, the results demonstrate the potential feasibility of an integrated AtJ-SAF facility processing 2,000 t day⁻¹ of wheat straw, supported by energy integration, co-product valorisation, and on-site production of enzymes, oxygen, and renewable hydrogen. Electrolysis provides over 5.8 t day⁻¹ of hydrogen to support downstream hydro-processing. Economically, the pathway yields a Minimum Jet Selling Price (MJSP) of £0.78–£2.05 kg⁻¹ SAF across the financing scenarios investigated. Although this remains above the assumed fossil jet-fuel price of approximately £0.45–£0.75 kg⁻¹, the results indicate potential for further cost reduction through process optimisation, economies of scale, favourable financing, and supportive policy mechanisms such as carbon pricing and SAF incentives.

Environmentally, the pathway achieves approximately 80% life-cycle GHG reduction relative to the fossil-kerosene benchmark (89 g CO₂-eq/MJ SAF) in line with UK SAF Mandate, demonstrating the potential of wheat-straw-derived AtJ-SAF to satisfy relevant UK sustainability requirements.

This performance is principally enabled using an agricultural residue, co-product valorisation, and integration of circular energy flows. The results therefore reinforce the potential environmental benefits of second-generation SAF pathways when integrated within resource-efficient systems.

The S-LCA provides a screening-level assessment of social risks across the SAF supply chain. Road transport accounted for the largest share of medium-risk hours (>40%), followed by SAF production and wheat cultivation, while fair salary emerged as a persistent indicator across the value chain. Within the foreground production supply chain, the UK *Collection, purification and distribution of water* sector was identified as a recurrent hotspot across several indicators. These findings demonstrate the value of MRIO-based S-LCA for early identification of potential social hotspots and for informing responsible sourcing, procurement, and supply-chain due diligence.

Sensitivity and uncertainty analyses further identify the principal factors influencing system performance. Operating expenditure, particularly feedstock, enzyme, and utility costs, exerts strong influence on MJSP, while Monte Carlo analysis indicates moderate uncertainty around the base-case estimate. Environmental sensitivity similarly identifies feedstock and chemical inputs as important contributors to GWP. Furthermore, increasing plant capacity from 1,000 to 4,000 t day⁻¹ reduces MJSP through economies of scale, although practical deployment remains constrained by regional feedstock availability, collection, and logistics. Collectively, these findings identify process efficiency, cost-effective feedstock sourcing, strategic scale selection, and supportive policy mechanisms as important determinants of commercial competitiveness.

By integrating technical, economic, environmental, and social assessments within a single framework, this research contributes a holistic evaluation of wheat-straw-derived AtJ-SAF and demonstrates the trade-offs and synergies that may be obscured when these dimensions are considered independently. The framework provides an evidence base for assessing whether

improvements in aviation decarbonisation can be achieved alongside economic viability, environmental integrity, and responsible supply-chain development.

Future research should prioritise pilot-scale validation of key conversion stages, catalyst durability under variable feedstock conditions, improved heat integration, and further optimisation of low-carbon hydrogen supply. Dynamic techno-economic models incorporating market volatility, policy incentives, and investment uncertainty would strengthen assessment of commercial deployment. Environmental assessment should further examine market-mediated feedstock displacement, soil-organic-carbon effects, and consequential impacts, while S-LCA should incorporate higher-resolution regional data, primary stakeholder evidence, and context-specific indicators. Integrating these advances within multi-objective optimisation frameworks would enable more robust assessment and design of commercially viable, environmentally sustainable, and socially responsible SAF systems.

CRedit authorship contribution statement

Chike Ucheana: Conceptualization, Formal analysis, Methodology, Software, Validation, Writing - original draft. **Maria Fernanda Rojas-Michaga:** Conceptualization, Methodology, Software, Investigation, Validation, Writing - review & editing. **Kevin J. Hughes:** Resources, Supervision, Writing - review & editing. **Derek Ingham:** Project administration, Resources, Supervision, Writing - review & editing. **Mohamed Pourkashanian:** Resources, Supervision, Writing - review & editing.

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.

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