Techno-economic and environmental impacts assessments of sustainable aviation fuel production from forest residue

Table S1: Breakdown of Direct fixed capital cost of SAF plant

Cost category	Estimation assumptions
Total equipment purchases cost (*PC*)	Sum of listed equipment purchases cost and unlisted equipment purchase cost
Process piping (a)	0.31 × *PC*[1]
Instrumentation (b)	0.13 × *PC*[1]
Insulation (c)	0.03 × *PC*[2]
Electrical (d)	0.10 × *PC*[1]
Buildings (e)	0.29 × *PC*[1]
Yard improvement (f)	0.10 × *PC*[1]
Auxiliary facilities (g)	0.20 × *PC*[1]
Installation (h)	0.50 × *PC*[2,3]
Total plant direct cost (TPDC)	*PC + a + b + c + d + e + f + g + h*
Engineering (i)	0.15 × *TPDC*[4]
Construction (j)	0.10 × *TPDC*[4]
Total plant other cost (TPOC)	*k*
Contingency (k)	0.1*(TDPC+TPIC)[5]
Direct fixed capital cost (DFC)	*DFC = TPDC + TPIC + TPOC*
Startup and validation cost	5% of *DFC*
Working capital	Operating cost for one month
Total investment (*TI*)	*DFC* + Startup cost + Working capital

Table S2. Catalyst Details

	Catalyst	Feed flow rate (L/H)	WHSV (Lgcat−1 h−1)	Catalyst req for 3 years (gm)	Cost/kg	Total cost per 3 year
Water Gas Shift Reaction	Cu-ZnO-Al2O3	38037962	15. 7[6]	2422800.00	5	12114
Fischer Tropsch Process	Cobalt	68058732	20[7]	3402936.6	18	61252.8
Hydrocraking (kg/hr)	0.5Pt/Y(100)35A	6957	2.3[8]	3024.782609	20	60495.6

FT Reactions

1. **Methane (CH_4)**: The formation of methane generally increases with temperature, which indicates a shift towards lighter hydrocarbons and possibly due to the hydrogenation of smaller intermediate carbon species.

   $CO+3H_2 \rightarrow CH_4+H_2OCO+3H_2 \rightarrow CH_4+H_2O$

2. **C_2-C_4 Hydrocarbons**: These include ethane, propane, and butanes. Their selectivity also tends to increase slightly at higher temperatures.

   $2CO+5H_2 \rightarrow C_2H_6+2H_2O_2CO+5H_2 \rightarrow C_2H_6+2H_2O$

   $3CO+7H_2 \rightarrow C_3H_8+3H_2O_3CO+7H_2 \rightarrow C_3H_8+3H_2O$

   $4CO+9H_2 \rightarrow C_4H_{10}+4H_2O_4CO+9H_2 \rightarrow C_4H_{10}+4H_2O$

3. **C_{5+} Hydrocarbons**: These are heavier fractions, including waxes and long-chain alkanes, which are more desirable for diesel and wax production. The selectivity towards C_{5+} hydrocarbons slightly decreases from 200 °C to 215 °C, reflecting a reduced chain growth probability at higher temperatures.

   $n\,CO + (2n+1)H_2 \rightarrow CnH_{2n+2} + nH_2O$

4. **C_5-C_{10} Hydrocarbons**

   These include lighter liquid fuels like gasoline components. The reaction can be generalized as:

   $nCO+(2n+1)H_2 \rightarrow C_nH_{2n}+2+nH_2OnCO+(2n+1)H_2 \rightarrow C_nH_{2n}+2+nH_2O$

   For n = 5 to 10:

   $5CO+11H_2 \rightarrow C_5H_{12}+5H_2O_5CO+11H_2 \rightarrow C_5H_{12}+5H_2O$(Pentane) $10CO+21H_2 \rightarrow C_{10}H_{22}+10H_2O_{10}CO+21H_2 \rightarrow C_{10}H_{22}+10H_2O$ (Decane)

5. **C_{11}-C_{18} Hydrocarbons**

   These are typically found in diesel and jet fuel ranges.

   $11CO+23H_2 \rightarrow C_{11}H_{24}+11H_2O_{11}CO+23H_2 \rightarrow C_{11}H_{24}+11H_2O$ (Undecane)

   $18CO+37H_2 \rightarrow C_{18}H_{38}+18H_2O_{18}CO+37H_2 \rightarrow C_{18}H_{38}+18H_2O$ (Octadecane)

6. **C_{19}-C_{34} Hydrocarbons**

   These heavier hydrocarbons are important for producing high-quality diesel and waxes.

   $19CO+39H_2 \rightarrow C_{19}H_{40}+19H_2O_{19}CO+39H_2 \rightarrow C_{19}H_{40}+19H_2O$ (Nonadecane)

$34CO+69H_2 \rightarrow C_{34}H_{70}+34H_2O_{34}CO+69H_2 \rightarrow C_{34}H_{70}+34H_2O$ (Tetratriacontane)

Table S3: Conversion factors and degree of removal of various compounds in the various processes

Process	Compound	Factor	Type	reference
Gas cleaning	H_2S, CO_2	Reduction to 0.1 ppm	Removal	[9]
Watergas shift reaction	CO	85	Conversion	[10]
Fischer-Tropsch synthesis	CO	98	Conversion	[11,12]
Hydrotreatment	C_{17+}	70	Yield	[8]

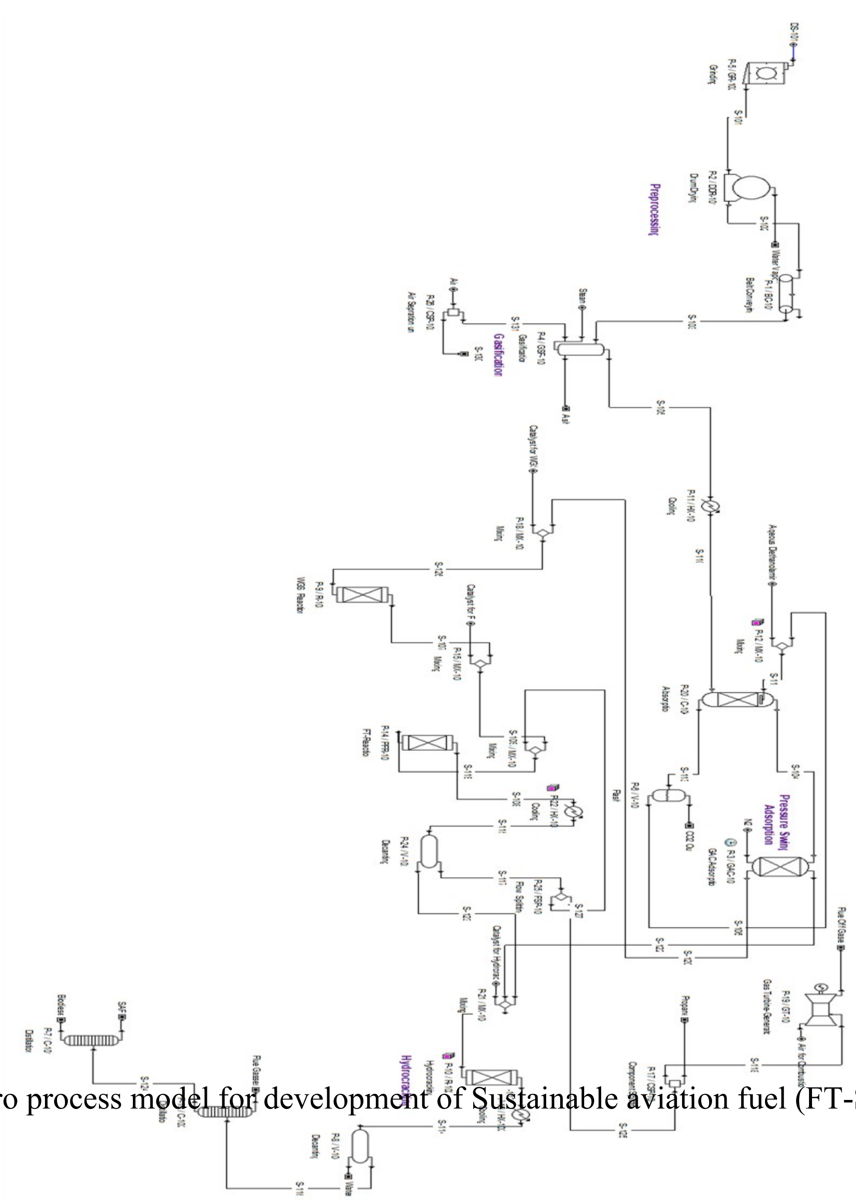

Fig S1: SuperPro process model for development of Sustainable aviation fuel (FT-SAF-SPK).

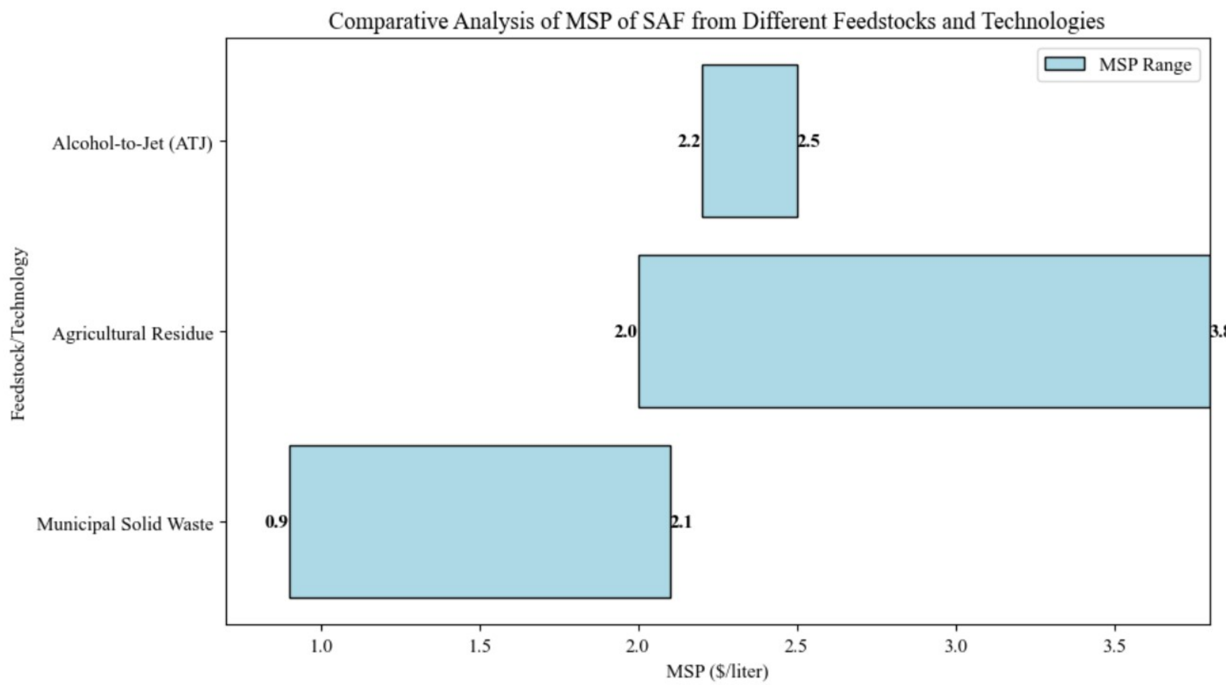

Fig S2: Comparative analysis of MSP of SAF

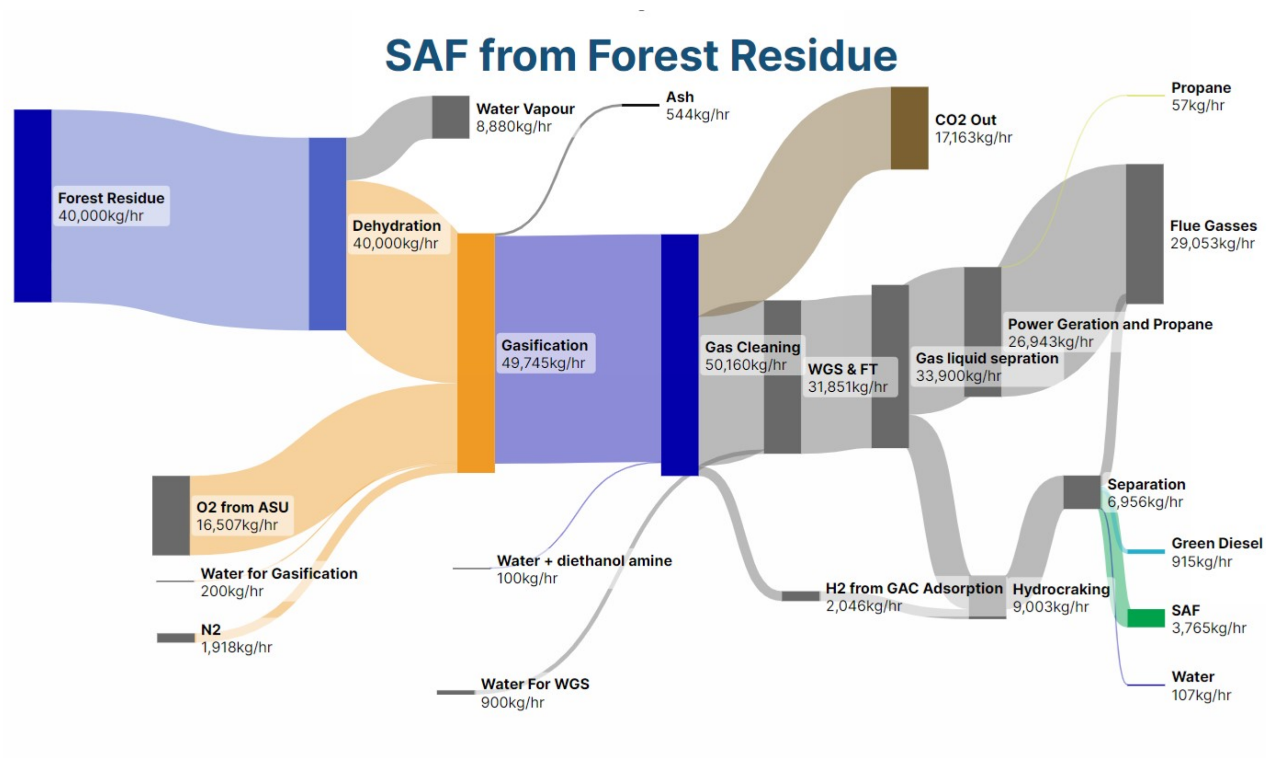

Fig S3: Net Mass Flows and Energy balance Sankey diagram.

Table S4: Cumulative Energy Demand

Impact category (Unit :MJ)	Total	Proxy_ Water, at user NREL/US U	Forest residue,	Diethanolamine	Steam, for chemical processes,	Diesel	Electricity Mix eGRIS 2022/US US-EI U	Disposal, liquid wastes, unspecified to waste water treatment/l NREL/RNA U	Disposal, wood ash mixture, pure, 0% water, to sanitary landfill/US * US-EI U	Proxy_Disposal, inert solid waste, to inert material landfill NREL/US U	Proxy_Disposal, heavy alkalide naphtha, to sanitary landfill NREL/US U
Total	2.08	0.00132	2.724	0.020	1.262	-0.28275	-1.668	0.000549	5.85E-04	0.008093	0.022
Non renewable, fossil	-0.086	0.00085	0.056	0.019	1.251	-0.27805	-1.166	0.000418	5.49E-04	0.007854	0.020
Non-renewable, nuclear	-0.375	0.00032	0.0009	0.001	0.0087	-4.0E-04	-0.384	9.92E-05	2.82E-05	0.000186	0.0015
Non-renewable, biomass	4.46E-07	4.84E-10	6.74E-08	8.7E-09	1.02E-06	-2.1E-09	-6.9E-07	3.89E-10	8.9E-10	1.33E-08	2.57E-08
Renewable, biomass	2.648	8.13E-05	2.666	0.0001	7.3E-04	-1.3E-04	-0.019	7.39E-06	2.26E-06	1.53E-05	1.01E-04
Renewable, wind, solar, geothermal	-0.067	3.52E-05	1.2E-05	0.0001	9.2E-04	-1.4E-04	-0.068	1.02E-05	2.72E-06	1.76E-05	1.69E-04
Renewable, water	-0.029	2.92E-05	0.0001	0.0001	8.43E-04	-3.7E-04	-0.030	1.44E-05	3.1E-06	2.03E-05	1.39E-04

Assumptions in soil carbon change calculations:

1. We used energy beneficial case in for production of SAF from forest residue to evaluate carbon change in soil. In previous study, Scenario 1, one hectare can produce approximately ~338.8. dry metric tons (Mg) of biomass over a 100-year period, suitable for biofuel production [13]. This calculation considers that 50% biomass is collectable for SAF production. This total is calculated based on repeating the 25-year rotation cycle four times, with each rotation producing 169.4 dry Mg ha^{-1} of biomass.
   The yield of SAF from dried biomass is ~13%, hence 338 dry metric ton biomass can produce 43.94MT of SAF. The greenhouse gas (GHG) emissions associated with producing 1 kg of Sustainable Aviation Fuel (SAF) from forest residue are approximately 24.56 g CO_2-eq/MJ. The 44MT of SAF will produce 1.1 MT CO_2 eq.
   The chemical composition and energy content per kilogram of SAF and conventional jet fuels are comparable, so they emit roughly the same amount of CO_2 when burned. Combustion of jet fuel releases about 3.15 kilograms of CO_2 per kilogram of fuel burned. SAF produced from biomass from one hectare over 100 hectors will produce 138.41-ton eq CO_2.

Table S4: Description of soil carbon dynamics calculations (values in tCO_2 eq)

	S1		
	All decay	Pile Burning	Biofuel
Biogenic Carbon Uptake by Logs	-923.0	-855.4	-855.4
Biogenic Carbon Uptake by Litter (Residues) and Residues for Biofuel/Pile Burning	-298.1	-276.1	-276.1
Biogenic Carbon Uptake by Litter (Litterfall)	-532.7	-532.7	-532.7
Biogenic Carbon Uptake by Litter (Roots)	-720.9	-720.9	-720.9
Forest Operations	15.2	14.5	15.5
Biofuel Production			1.1
Biofuel transportation and combustion			140.5
Pile burning		145.1	
Emissions from litter and mineral soil	1543.3	1397.0	1397.0
Total	-916.2	-828.5	-831

In calculation of net CO_2 removal we consider life cycle CO2 emissions by transportation and combustion stage is 0.8gCO_2e/MJ and 73.2 gCO_{2e}/MJ[14,15]. Hence, 44 MT produces 1.5 MT of CO2 eq from transportation and ~139 MT eq of CO_2 emissions from combustion, total of 140.5ton eq CO_2.

References:

1 A. C. Dimian, Ed., in *Computer Aided Chemical Engineering*, Elsevier, 2003, vol. 13, pp. 571–604.
2 S. H. Mousavi-Avval and A. Shah, *Renewable and Sustainable Energy Reviews*, 2021, **149**, 111340.
3 M. Fernanda Rojas Michaga, S. Michailos, M. Akram, E. Cardozo, K. J. Hughes, D. Ingham and M. Pourkashanian, *Energy Conversion and Management*, 2022, **255**, 115346.
4 M. Finkelstein, B. H. Davison and J. D. McMillan, *Biotechnology for Fuels and Chemicals: The Twenty-Third Symposium*, Springer Science & Business Media, 2012.
5 S. H. Mousavi-Avval, S. Khanal and A. Shah, *Sustainability*, 2023, **15**, 10589.
6 Z. Li, N. Li, N. Wang, B. Zhou, J. Yu, B. Song, P. Yin and Y. Yang, *RSC Adv*, **12**, 5509–5516.
7 C. Niu, M. Xia, C. Chen, Z. Ma, L. Jia, B. Hou and D. Li, *Applied Catalysis A: General*, 2020, **601**, 117630.
8 S. Mitsuoka, K. Murata, T. Hashimoto, N. Chen, Y. Jonoo, S. Kawabe, K. Nakao and A. Ishihara, *ACS Omega*, 2024, **9**, 3669–3674.
9 Simultaneous Absorption of CO2 and H2S Into Aqueous Blends of N-Methyldiethanolamine and Diethanolamine | Environmental Science & Technology, https://pubs.acs.org/doi/10.1021/es0606475, (accessed May 9, 2024).
10 P. Spath, A. Aden, T. Eggeman, M. Ringer, B. Wallace and J. Jechura, *Biomass to Hydrogen Production Detailed Design and Economics Utilizing the Battelle Columbus Laboratory Indirectly-Heated Gasifier*, National Renewable Energy Lab. (NREL), Golden, CO (United States), 2005.
11 K. Im-orb, L. Simasatitkul and A. Arpornwichanop, *Energy*, 2016, **94**, 483–496.
12 N. Lümmen and E. Røstbø, *Energy*, 2020, **211**, 118996.
13 Soil organic carbon change can reduce the climate benefits of biofuel produced from forest residues - ScienceDirect, https://www.sciencedirect.com/science/article/pii/S2542435123005378, (accessed April 13, 2024).
14 Understanding variability in petroleum jet fuel life cycle greenhouse gas emissions to inform aviation decarbonization | Nature Communications, https://www.nature.com/articles/s41467-022-35392-1, (accessed April 15, 2024).
15 E. Yoo, U. Lee and M. Wang, *ACS Sustainable Chem. Eng.*, 2022, **10**, 8725–8732.