

Appendices

Appendix A:

A.1: Assumptions in Mannion et al. Model:

- [A.1] The initial feedstock is defined as 100kg in mass. If the mass is increased, the efficiency the system increases as heat losses are minimised. In all other cases total mass is arbitrary as emissions are normalised per MJ of SAF produced. This is a reasonable assumption.
- [A.2] Chemical reactions are 100% converted in the forward reaction rate for the full reaction mechanism, unless stated otherwise.
- [A.3] The energy consumed due to loss of heat and maintaining the fuel at constant temperature is contained within the system efficiency parameter. Here, the specific energy calculated is multiplied by 33% efficiency parameter to account for this loss.
- [A.4] The SAF energy density is set to be in the range of the ASTM 7566 Standard minimum and reported LHV for UOP HEFA of 42.8-43.9 MJ/kg. The chosen SAF energy density/ lower heating value is 43.744 MJ/kg from literature measurements of used cooking oil derived HEFA/HRJ [1].
- [A.5] The fuel production facility is assumed to be in Finland, with electricity from the main grid as a source of energy. This emission factor associated with electricity utilisation uses an average GHG intensity based on Finland's electricity production facilities from [2] (mix of renewables and fossil fuels).
- [A.6] Fuel production is assumed to use 100% electricity as energy source for default scenario (Scenario 3). This is not evidenced. No fossil fuels or waste is burned on site to produce on site-electricity. It is sourced directly from the grid.
- [A.7] The used cooking oil is filtered in 2 Stages. 1. Heating the used cooking oil from 25-35 C and pouring through a fine mesh to remove large particles. 2. Heating to 60 C and retaining for 30 minutes to remove water. It is then left to settle for 24 hours.
- [A.8] The used cooking oil is assumed to have a composition of 79.1% triglycerides, 1.8% diglycerides, 2.2 % monoglycerides, and 16.9% free fatty acids. Of the triglycerides, the composition is assumed to be 32.8% triolein, 6.5% tripalmitin, and 60% trilinolein [3, 4].
- [A.9] For hydrogenation, it is assumed that hydrogen is added in excess by a factor of ~35% of the mass needed to perform the hydrogenation. This excess hydrogen is assumed to be recovered and recycled back into the system; therefore excess hydrogen does not add to CO₂e count.
- [A.10] The initial feedstock is heated from 25 C to 420 C in the hydrocracking bath. (Based on the range of 350-450 C from literature) [4].
- [A.11] The size of the reaction chamber is set to these values. This is for heat loss calculations. The same sizing parameters are used for all fuel production baths. (This is a separate attempt at more accurate heat loss calculations, future work, not used in the current methodology)
- [A.12] Hydrocracking occurs at 420 C.
- [A.13] Only propane is removed at the propane cleave step. This is not evidenced.
- [A.14] CO₂ produced in the reaction process is captured directly from bath. It still contributes to the overall CO₂ cost.
- [A.15] Propane is purified using literature data for Naphtha purification. This is not evidenced.

- [A.16] Naphtha, propane, and other gases are separated and purified maintaining heat and not cooling. More information is needed. This is not evidenced.
- [A.17] Hydrogen used in fuel production is produced through steam methane reforming (SMR) which contributes its own intrinsic CO₂ cost.
- [A.18] The fuel production system is a batch production method.
- [A.19] There are no mass losses or residues left over in each reaction chamber. All elemental mass is conserved. This is not evidenced.
- [A.20] All chemical reactions are assumed to occur in one vessel, in a batch configuration according to the reaction mechanism given in Appendix B.
- [A.21] Unknown triglycerides, diglycerides, and monoglycerides in fuel mixture are converted to analogous forms of carboxylic acids and follow the analogous reaction mechanism.
- [A.22] As propane, water, CO & CO₂ are produced by the reaction mechanism by known molecules, the unknown molecules produce the same products, the change in mass% of reactants to products is observed for known reactions and applied to the unknowns.
- [A.23] Reaction mechanism is not specified based on structural isomers, it is simplified by describing only normal alkane products, knowing that any structural isomers will follow the same mass flow. The isomerisation is applied after the conclusion of the reaction mechanism, and after cracking. 83% of the n-alkanes are isomerised, and 17% remain n-alkanes, by experimental data [5].
- [A.24] 85% of the oleic acid is converted to stearic acid, 15% remains as oleic acid, as is defined by [4].
- [A.25] Consumption of stearic, oleic, and palmitic acid is assumed to occur by three processes (Decarboxylation, Decarbonylation, Hydrodeoxygenation) 0.68/0.03/0.29 by mass [6].
- [A.26] Energy calculation for hydrotreatment is calculated on specific heat capacity of heating known mass of triolein, trilinolein, and tripalmitin from 25-420 C. The reactions are mostly exothermic, hence any other energy required for the reactions to occur is taken internally.

Appendix B

All equations used in this work:

B.1: Energy Equations

The individual energy values for each production step are calculated separately as each production step contains a different molecular mixture and is fundamentally different. The energy calculations use scientific properties of the molecules in these fuel mixtures, and each energy calculation contains sourced academic literature information to provide accuracy and credibility to the calculation [4, 7-12]. The sum of the individual energies for each processing step is then the total energy use in conversion.

Below are the equations involved in the energy calculations.

The net energy E_{Net} (J) is described in Equation B.1. This is the total energy required for total conversion of used cooking oil to SAF and co-products.

$$E_{Net} = E_{Total} / \eta_{System} \quad \#(Equation B. 1)$$

Where η_{System} is the system efficiency to account for energy loss due to heat/friction/etc. Heat is assumed to be the primary method of energy loss. This is because of the heat loss calculation method. In the current methodology, the used cooking oil is heated to 400 C and maintained at 33% efficiency. It is assumed here that this low efficiency accounts for the energy that would be required to heat the fuel mixture. For more specific heat loss calculations see Equations B.7-B.13. These equations describe the total energy required to keep the fuel at constant temperature throughout the production process, $E_{Heating}$ (J). To reduce complexity and unnecessary uncertainty, Equations B.7-B.13 are not used in the current model, however, they describe a methodology to be used in the future for more accurate heat loss calculations.

The total energy use, E_{Total} (J), is the sum of each energy used in each of the processing steps in the feedstock to fuel conversion.

$$E_{Total} = E_{Filtration} + E_{Initial\ Hydropretreatment} + E_{Propane\ Cleave} + E_{Deoxygenation} + E_{Vapour-Liquid\ Separation} + E_{Second\ Hydro} \quad \#(Equation B. 2)$$

The energy required for filtration, $E_{Filtration}$ (J) is described as the energy required to heat the used cooking oil before mesh filtration, and energy required for water removal. It is assumed the used cooking oil is 100 kg in mass. The used cooking oil is initially heated from 25 C to 35 C to allow for good flow in mesh filtration. This removes large unwanted particles from the used cooking oil. Secondly, the used cooking oil is heated and retained at 100 C for 30 minutes to remove water. The energy required for filtration can therefore be described as:

$$E_{Filtration} = E_{Triolein} + E_{Trilinolein} + E_{Tripalmitin} + E_{Unknowns} \quad \#(Equation B. 3)$$

where the energies are dependent on the specific heat capacity of each molecule, e.g.,

$$E_{Triolein} = m_{Triolein} C_{p_{Triolein}} (T_f - T_i) \quad \#(Equation B. 4)$$

Where E (J) is the energy used, m (kg) is the mass, C_p (J/mol K⁻¹) is the specific heat capacity of the liquid, T_i (C) is the initial temperature, and T_f (C) is the final temperature. Equation B.4 is used to calculate the energies for each molecule in Equation B.3. $E_{Unknowns}$ (J) uses an average specific heat capacity of the molecules present in used cooking oil in Equation B.4. The mass proportions found in

Sotelo-Boyás et al [4] describe the mass% of each triolein, trilinolein, tripalmitin, and unknowns in used cooking oil.

The heat capacities of the are from Morad [8]. The specific heat capacity at liquid phase, C_p , (J/mol K⁻¹) was calculated using the Rowlinson-Bondi equation, and the procedure followed in Morad et al [8].

The initial hydrotreatment energy, $E_{Initial\ Hydrotreatment}$ (J), follows the same methodology as $E_{Filtration}$ (J), with separate assumptions. It is assumed that 100 kg of used cooking oil enters the reaction chamber at 25 C, and is heated to 400 C [4, 13].

Equation B.5 describes the energy used in removing propane from the reaction chamber, $E_{Propane\ Cleave}$ (J).

$$E_{Propane\ Cleave} = r_{VL} \left(m_{C_3H_8} + m_{C_3H_8\ Unknown} \right) \#(Equation\ B.\ 5)$$

Here r_{VL} (kJ/kg) is the rate of energy use in removing gas from a vapor-liquid reaction chamber, calculated by Zhang et al [12], $m_{C_3H_8}$ (kg) is the known mass of propane in the reaction chamber, derived from the reaction mechanism, and $m_{C_3H_8\ Unknown}$ (kg) is the mass of the estimated propane produced from unknowns in the reaction chamber. It is assumed here that the unknowns in the original feedstock mixture (21% of total) follow a similar reaction mechanism to the one described in section B.1 as they are similar molecules. Therefore, it is assumed that a certain percentage of the unknowns mass is converted to propane, water, etc. For calculating unknown propane, the relative mass of propane created compared to original known mass of triglyceride is calculated and applied to the unknowns. This method is then used for other estimations of unknown mass products such as water.

Equation 3.6 describes the standard enthalpy of reaction (kJ/mol).

$$\Delta_{Reaction} H = \sum v \Delta_{formation} H(products) - \sum v \Delta_{formation} H(reactants)$$

#(Equation B. 6)

Where v (mol) is the molarity in balanced chemical equation, and $\Delta_{formation} H$ (kJ/mol) is the formation enthalpy of the products and reactants. This calculation concluded that the overall reactions contribute negative enthalpy of formation, making the reactions overall exothermic. This provided motivation for the modelling of heat exchanges to better describe heat loss and to retain the reaction chamber at the desired temperature.

From here, it was modelled that heat exchangers are used to keep the reaction chambers at 400 C. Newtons law of cooling (Equation B.7) was used to estimate the typical heat loss of a reaction chamber 3 m high with a radius of 0.5 m and 0.01 m thick made from stainless steel with 0.1 m wool insulation. The sizes outlined above are the default sizes used for each reaction chamber in the modelled system. These diameters were chosen as it is typical for a cylindrical chamber in a fuel production facility to have a 3:1 ratio of height to diameter.

Newtons law of cooling, shown in Equation B.7, describes the heat lost (Q (J/s)) between a liquid fuel and its environment.

$$Q = hA(T_{fuel} - T_{env}) \#(Equation B. 7)$$

Where,

$$h = \frac{q}{\Delta T} \#(Equation B. 8)$$

Here, A (m^2) is the surface area of the container, T_{fuel} (C) is the temperature of the fuel, T_{env} (C) is the temperature of the environment, and h ($W/m^2/K$) is the heat transfer co-efficient. q is the heat flux (W/m^2), and ΔT (C) is the difference in temperature between a solid surface and surrounding fluid. h is different for each material, so a combination of the heat co-efficient of the fuel mixture is needed. Palmitic and oleic acid's heat transfer coefficients were chosen to represent the fuel as they are well thermodynamically studied [14].

$$\frac{1}{h} = \frac{1}{h_{Trilinolein}} + \frac{1}{h_{Heptadecane}} \#(Equation B. 9)$$

If we assume there is little difference between the temperature of the liquid fuel and the surrounding solid material, we can say:

$$h \cong q \#(Equation B. 10)$$

And therefore,

$$\frac{1}{q} = \frac{1}{q_{Trilinolein}} + \frac{1}{q_{Heptadecane}} \#(Equation B. 11)$$

And,

$$Q = qA(T_{fuel} - T_{env}) \#(Equation B. 12)$$

The energy, $E_{Heating}$ (J) is calculated by:

$$E_{Heating, Processing Step} = Qt = qA(T_{fuel} - T_{env})t \#(Equation B. 13)$$

Where t (seconds) is the total time of reaction, and "Processing Step" defines which processing step's heating energy is being calculated.

This equation is used to describe the energy needed to maintain a constant temperature of 400 C for each step in the production process. In each case where heating is needed, $E_{Heating, Processing Step}$ is added to the final energy. For example:

$$E_{Propane\ Cleave} = r_{VL} \left(m_{C_3H_8} + m_{C_3H_8\ Unknown} \right) + E_{Heating, Propane\ Cleave} \quad \#(Equation\ B.\ 14)$$

In the processing steps Deoxygenation, Second Hydrotreatment, Fractional Distillation 1, and Fractional Distillation 2, the energy used to maintain 400 C is the total energy used for this processing step.

In the current methodology, the heating calculations in Equations B.7-B.13 add too much unnecessary uncertainty to the heat loss calculation as the size of the reaction chambers, times of processing steps, and other factors are all individually assumed. Therefore, it is assumed that when the used cooking oil is initially heated in the initial hydrotreatment processing step, it does not cool. The heat loss for the entire system is therefore accounted for by adding the efficiency term in Equation B.1, and for processing steps that only require heating; Deoxygenation, Second Hydrotreatment, Fractional Distillation 1, and Fractional Distillation 2, the energy becomes zero. This does not mean the energy that would be required to maintain the fuel mixture at 400 C in these steps is ignored but is accounted for by one assumption in Equation B.1. With more information from industry, the model can be improved by using Equations B.7-B.13 in future.

The energy for vapor-liquid separation, $E_{Vapor-Liquid\ Separation}$ (J), is shown in Equation B.15. CO₂, CO, H₂, H₂O, and C₃H₈ are produced through the reaction mechanism described in Appendix B. The CO₂, m_{CO_2} (kg), is assumed to be separated and captured, while the other gases are assumed to be separated and stored. The energy cost for removing and capturing carbon is higher than the energy cost from only removing and storing the gas.

$$E_{Vapor-Liquid\ Separation} = r_{CO_2} \left(m_{CO_2} \right) + r_{VL} \left(m_{CO} + m_{H_2O} + m_{C_3H_8} + m_{H_2} \right) \quad \#(Equation\ B.\ 15)$$

Where r_{CO_2} (kJ/kg) is the rate of energy use for vapor-liquid separation for CO₂, r_{VL} (kJ/kg) is the rate of energy use for vapor-liquid separation defined in Equation B.5, and $m_{Molecule}$ (kg) is the mass of the various molecules. CO₂ has a separate rate of energy use as in Zhang et al [12] compared to the other gases as CO₂ uses more energy per kg due to the energy required in carbon capture and storage. It is assumed that the intrinsic CO₂ in the overall fuel production process is captured and not released.

Naphtha is produced when larger chain alkanes are cracked to shorter chain alkanes. Equation B.16 describes the total mass and composition of Naphtha, $m_{Naphtha}$ (kg). The naphtha must then be purified. The energy use in naphtha purification is defined according to Equation B.17.

$$m_{Naphtha} = m_{C_8H_{18}} + m_{C_7H_{16}} + m_{C_6H_{14}} \quad \#(Equation\ B.\ 16)$$

$$E_{Naphtha\ Purification} = p_N \times m_{Naphtha} \quad \#(Equation\ B.\ 17)$$

here, p_N (kJ/kg) is the energy required for purification [10]. This energy consumption is defined for naphtha purification specifically. It is currently used in the case propane purification, in the assumption that purification of other gases requires similar energy (Equation B.19).

Similarly, the mass of the propane formed in the reaction mechanism is described in Equation B.18, and the energy use in propane purification is defined in Equation B.19.

$$m_{Propane} = m_{C_3H_8} + m_{C_3H_8\ Unknown} \quad \#(Equation\ B.\ 18)$$

$$E_{Propane\ Purification} = p_N \times m_{Propane} \quad \#(Equation\ B.\ 19)$$

The residual fuel burning energy, $E_{Residual\ Fuel\ Burning}$ (J) is set to zero. It is assumed here that there is no mass loss in any process in the feedstock to fuel conversion, and there are no trace liquids left in the container. Hence, there is no waste fuel to burn.

The net energy use in fuel production, E_{Net} (J), then needs to be converted to gCO₂e/MJ_{SAF}. Firstly, the definition of this energy is the energy required to convert 100 kg of used cooking oil to SAF and other products. The term gCO₂e/MJ_{SAF} is the standard value used in SAF LCA and is defined as the total gCO₂e per MJ of SAF produced. Therefore, we need to consider the yield of SAF, $Yield_{SAF}$ (kg SAF/ kg used cooking oil), and the lower heating value, LHV_{SAF} (MJ/kg), /energy density of the produced SAF. The LHV_{SAF} (MJ/kg) is set to a measured used cooking oil hydroprocessed renewable jet LHV above the ASTM LHV legal minimum standard [1]. Next, we need to consider the source of this energy. From before, the total energy of production is assumed to be sourced from 100% electricity. Hence, the emission factor of the electric grid, EF_{grid} , must be considered. This is set to the average grid gCO₂e/MJ for electricity consumption in Finland, as we assume the fuel production facility is in Finland.

B.2: Conversion Equations

The LHV_{SAF} (MJ/kg) is set to a measured used cooking oil hydroprocessed renewable jet LHV above the ASTM LHV legal minimum standard [1]. Next, we need to consider the source of this energy.

From before, the total energy of production is assumed to be sourced from 100% electricity. Hence, the emission factor of the electric grid, EF_{grid} , must be considered. This is set to the average grid gCO_2e/MJ for electricity consumption in Finland.

$$E_{Net} \frac{[MJ]}{[100 \text{ kg UCO}]} \rightarrow \frac{E_{Net}}{Yield_{SAF}} \frac{[MJ]}{[100 \text{ kg UCO}]} \frac{[100 \text{ kg UCO}]}{[kg SAF]} \rightarrow \frac{E_{Net}}{Yield_{SAF} \times LHV_{SAF}} \frac{[MJ][kg SAF]}{[kg SAF][MJ]} \rightarrow \left(\frac{E_{Net}}{Yield_{SAF} \times LHV_{SAF}} \right) \times EF_{grid} [gCO_2e/MJ] \\ = Total \text{ } gCO_2e/MJ_{SAF} \text{ from energy use} \# (Formula B. 20)$$

Intrinsic CO_2 is formed as part of the reaction mechanism in Appendix B. Like how the energy is standardized in Formula B.20, the intrinsic CO_2 must be converted to gCO_2e/MJ_{SAF} .

$$CO_{2 \text{ Intrinsic}} \frac{[g \text{ } CO_2]}{[100 \text{ kg UCO}]} \rightarrow \frac{CO_{2 \text{ Intrinsic}}}{Yield_{SAF}} \frac{[g \text{ } CO_2]}{[100 \text{ kg UCO}]} \frac{[100 \text{ kg UCO}]}{[kg SAF]} \rightarrow \frac{CO_{2 \text{ Intrinsic}}}{Yield_{SAF} \times LHV_{SAF}} \frac{[g \text{ } CO_2][kg SAF]}{[kg SAF][MJ]} \\ = Total \text{ } gCO_2e/MJ_{SAF} \text{ from intrinsic } CO_2 \# (Formula B. 21)$$

Hydrogen is consumed as part of the reaction mechanism in Appendix B. The production of this hydrogen is considered in the LCA of the SAF production. Like the Formula B.20 and B.21, the total hydrogen use must be standardized:

$$H_2 \frac{[kg]}{[100 \text{ kg UCO}]} \rightarrow \frac{H_2}{Yield_{SAF}} \frac{[kg \text{ } H_2]}{[100 \text{ kg UCO}]} \frac{[100 \text{ kg UCO}]}{[kg SAF]} \\ \rightarrow \frac{H_2}{Yield_{SAF} \times LHV_{SAF}} \frac{[kg \text{ } H_2][kg SAF]}{[kg SAF][MJ]} \\ \rightarrow \left(\frac{H_2}{Yield_{SAF} \times LHV_{SAF}} \right) \times EF_{Hydrogen \text{ Production}} \frac{[kg \text{ } H_2]}{[MJ]} \left[\frac{g \text{ } CO_2e}{kg \text{ } H_2} \right] \\ = Total \text{ } gCO_2e/MJ_{SAF} \text{ from hydrogen use} \# (Formula B. 22)$$

Here, $EF_{Hydrogen \text{ Production}}$, is the emission factor for hydrogen production from steam methane reforming (SMR) [15], known as grey hydrogen. The total gCO_2e/MJ_{SAF} for fuel production is calculated by the Equation B.23. Note here, the emission factor for different methods of hydrogen production can easily be replaced to simulate more sustainable hydroprocessed renewable jet fuel production methods.

$$Total \text{ } CO_2e/MJ = \\ Total \text{ } gCO_2e/MJ_{SAF} \text{ from energy use} + Total \text{ } gCO_2e/MJ_{SAF} \text{ from intrinsic } CO_2 \\ + Total \text{ } gCO_2e/MJ \text{ from hydrogen use} \# (Equation B. 23)$$

The total gCO_2e/MJ is the total CO_2 equivalent to make all end products. This is the final LCA value with no allocation methods.

B.3: Allocation Equations

Equations B.24 and B.25 show the energy and mass allocation methodology used this paper.

$$GHG_{Energy Allocation} = Total\ gCO_2e/MJ\ [gCO_2e/MJ] \times \left(\frac{m_{SAF} \times LHV_{SAF} [MJ]}{Total\ E\ [MJ]} \right)$$

#(Equation B. 24)

$$GHG_{Mass Allocation} = Total\ gCO_2e/MJ\ [gCO_2e/MJ] \times \left(\frac{m_{HRJ} [kg]}{Total\ m\ [kg]} \right)$$

#(Equation B. 25)

where,

$$Total\ E\ [MJ] = m_{Naphtha} * LHV_{Naphtha} + m_{SAF} * LHV_{SAF} + m_{Diesel} * LHV_{Diesel} + m_{Propane} * LHV_{Propane}$$

#(Equation B. 26)

and,

$$Total\ m\ [kg] = m_{Naphtha} + m_{SAF} + m_{Diesel} + m_{Propane} \#\#$$

#(Equation B. 27)

For Displacement:

$$GHG_{Displacement} = Total\ gCO_2e/MJ\ [gCO_2e/MJ] - (m_{Naphtha} * EF_{Naphtha} + m_{Diesel} * EF_{Diesel} + m_{Propane} * EF_{Propane})$$

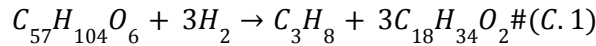
#(Equation B. 24)

Appendix C

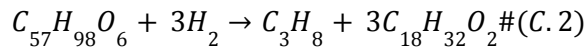
C.1: Full Triglyceride reaction mechanism for this work:

Formation of fatty acids:

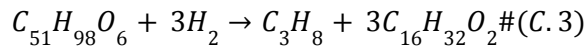
Triolein + Hydrogen → Propane + Oleic acid



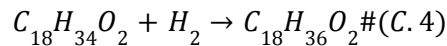
Trilinolein + Hydrogen → Propane + Linoleic acid



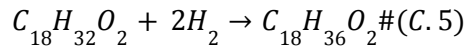
Tripalmitin + Hydrogen → Propane + Palmitic acid



Oleic acid + Hydrogen → Stearic acid

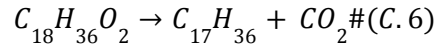


Linoleic acid + Hydrogen → Stearic acid

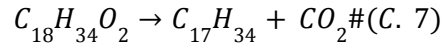


Decarboxylation reactions:

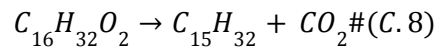
Stearic acid \rightarrow Heptadecane + Carbon Dioxide



Oleic acid \rightarrow Heptadecene + Carbon Dioxide

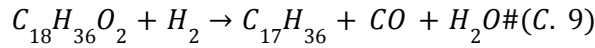


Palmitic acid \rightarrow Pentadecane + Carbon Dioxide

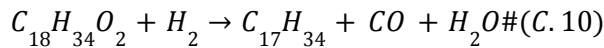


Decarbonylation reactions:

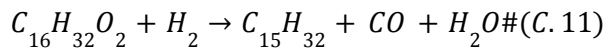
Stearic acid + Hydrogen \rightarrow Heptadecane + Carbon monoxide + Water



Oleic acid + Hydrogen \rightarrow Heptadecene + Carbon monoxide + Water

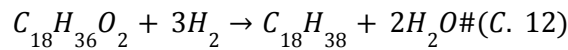


Palmitic acid + Hydrogen \rightarrow Pentadecane + Carbon monoxide + Water

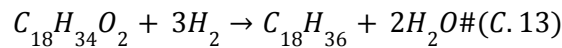


Hydrodeoxygenation reactions:

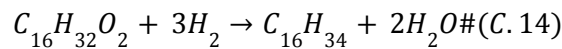
Stearic acid + Hydrogen \rightarrow Octadecane + Water



Oleic acid + Hydrogen \rightarrow Octadecane + Water



Palmitic acid + Hydrogen \rightarrow Hexadecane + Water



C.2: Effect of Decarbonisation Pathway on the LCA value:

Table 1 shows the effect of decarbonization pathway. Clearly, the lowest emissions arise when the reaction is pushed towards decarbonylation. This lowers the lifecycle fuel production emissions by lowering the amount of CO₂ produced. As well as that, the decarbonylation pathway uses less hydrogen than the hydrodeoxygenation pathway. The catalyst used can therefore change the overall LCA value, as it changes the mass proportions of the decarbonization pathway. In this study, a NiMo catalyst is used, with the mass proportions observed as 68% decarboxylation, 3% decarbonylation, and 29% hydrodeoxygenation reactions, by Chu et al [6]. This is the default proportions in the mass balance.

Table 1: Effect changing decarbonisation pathway in the reaction mechanism in C.1 has on individual greenhouse gas contributions for each step in production, total production emissions, total hydrogen consumed, and total intrinsic CO₂ produced. Stearic acid, oleic acid, and palmitic acid have a known mass before decarbonisation takes place. The different sections in “Energy Allocation Result” change how this mass is proportioned between the different decarboxylation, decarbonylation, and hydrodeoxygenation pathways in C.1. The default results show mass proportions for all acids to be decarbonised through 68% decarboxylation, 3% decarbonylation, and 29% hydrodeoxygenation reactions. The decarboxylation result shows

Production Process	Energy Allocation Result				Units
	Default	Decarboxylation	Decarbonylation	Hydrodeoxygenation	
Filtration	0.26	0.26	0.26	0.25	gCO ₂ e/MJ _{SAF}
Initial Hydrocracking	0.68	0.69	0.70	0.66	gCO ₂ e/MJ _{SAF}
Propane Cleave	0.10	0.10	0.10	0.10	gCO ₂ e/MJ _{SAF}
Deoxygenation	0.17	0.17	0.17	0.16	gCO ₂ e/MJ _{SAF}
Vapour-Liquid Separation	1.47	1.81	1.03	0.78	gCO ₂ e/MJ _{SAF}
Propane Purification	0.10	0.11	0.11	0.10	gCO ₂ e/MJ _{SAF}
Second Hydrotreatment	0.17	0.17	0.17	0.16	gCO ₂ e/MJ _{SAF}
Fractional Distillation 1	0.17	0.17	0.17	0.16	gCO ₂ e/MJ _{SAF}
Fractional Distillation 2	0.17	0.17	0.17	0.16	gCO ₂ e/MJ _{SAF}
Naphtha Purification	0.74	0.74	0.74	0.74	gCO ₂ e/MJ _{SAF}
Intrinsic CO ₂	2.64	3.95	0.00	0.00	gCO ₂ e/MJ _{SAF}
Hydrogen Production	5.87	4.50	6.03	8.90	gCO ₂ e/MJ _{SAF}
Total Emissions	12.56	12.86	9.66	12.18	gCO ₂ e/MJ _{SAF}
Hydrogen consumed	2.71	2.04	2.73	4.25	kg
CO ₂ produced	10.32	15.19	0.00	0.00	kg

Appendix D: Data used in this work

Appendix D.1: General Data

Data for Fuel Production						
		Specific Data for Fuel Production	Unit	Data	Ref	Comment/Notes/Explanations
Fuel Properties		Feedstock to Fuel Conversion Yield	mass%	47%	Mannion et al.	
		SAF Energy Density	MJ/kg	43.744	[1, 16]	42.8 = ASTM D 7566 min.
Default Emission Factors for Stationary Combustion In The Energy Industries	Coal	Emission Factor	kgCO ₂ /TJ	98300.00	[17]	This section uses data from the 2006 IPCC Greenhouse Gas Inventories [48] to estimate the emissions from coal use, natural gas use, and gas/diesel oil use. Currently, these values are not being used as 100% of the energy use in production is accredited to electricity, this is "Case 1".
		CH ₄ Content	kgCH ₄ /TJ	1.000	[17]	
		N ₂ O Content	kgN ₂ O/TJ	1.500	[17]	
	Natural Gas	Emission Factor	kgCO ₂ /TJ	56100.00	[17]	
		CH ₄ Content	kgCH ₄ /TJ	1.000	[17]	
		N ₂ O Content	kgN ₂ O/TJ	0.100	[17]	
	Gas/Diesel Oil	Emission Factor	kgCO ₂ /TJ	74100.00	[17]	
		CH ₄ Content	kgCH ₄ /TJ	3.000	[17]	
		N ₂ O Content	kgN ₂ O/TJ	0.600	[17]	
Global Warming Potentials		CO ₂	gCO ₂ e	1.000	[18]	These values are needed to convert the CO ₂ , CH ₄ , and N ₂ O content into CO ₂ e.
		CH ₄	gCO ₂ e	25.000	[18]	
		N ₂ O	gCO ₂ e	298.000	[18]	
		GHG Emission Factor for Electricity Consumption - Finland	tCO ₂ e /MWh	0.077	[2]	The model uses Finland as base of operation for fuel production
% Share of Energy in HEFA Production as:		Electricity	%	100	Mannion et al.	The total energy use is split amongst these shares and the emissions are calculated according to the emission factors shown in "Default Emission Factors for Stationary Combustion in The Energy Industries"
		Coal	%	0	Mannion et al.	
		Natural Gas	%	0	Mannion et al.	

	Petroleum	%	0	Mannion et al.	
Sunflower Oil Typical Composition	Triglyceride Composition	wt%	79.10	[4]	Triglycerides are modelled with reaction mechanism
	Diglyceride Composition	wt%	1.80	[4]	
	Monoglyceride Composition	wt%	2.20	[4]	
	Free Fatty Acid Composition	wt%	16.90	[4]	
Sunflower Oil Triglyceride Composition	Palmitic Composition	wt%	6.50	[4]	0.7% remaining mass% is contained in the model - it is treated as unknown triglycerides and is treated the same as the unknowns with the unknown diglycerides, monoglycerides, and free fatty acids
	Stearic Composition	wt%	5.80	[4]	
	Oleic Composition	wt%	27.00	[4]	
	Linoleic Composition	wt%	60.00	[4]	
Purification Energy Cost	Removal Of CO ₂	MJ/kg	5.45	[12]	Modelled as CO ₂ separation from fuel mix (MEA Capture)
	Removal Of Any Gas	MJ/kg	1.47	[12]	Modelled as CO ₂ separation from fuel mix (no MEA Capture)
	Naphtha Purification	kg/1.5kJ	0.001	[10]	from GREET paper
Temperatures of reactors	Initial Hydrotreatment Temperature	C	400.00	[4]	Based on the range of 350-450 C from literature
	Typical Hydrodeoxygenation Conditions	deg C	400.00	[4]	Based on the range of 320-420 C from literature
Hydrogen Production	Emissions Factor (Steam Methane Reforming Process)	kg CO ₂ e /kg H	8.47	[19]	Hydrogen used in fuel production has intrinsic CO ₂ in its own production The total emissions here can be reduced if green hydrogen is used
	Emissions Factor (Electrolysis by Renewable Energy)	kg CO ₂ e /kg H	1.57	[20]	

Appendix D.2: Property Data

D.2.1: Triglycerides and Free Fatty Acids for Heat Calculations

Molecule	Heat capacity (KJ/Kg K)	Reference
Triolein	2.08	[8]
Trilinolein	2.01	[9]
Tripalmitin	2.18	[8]
Oleic acid	2.31	[9]
Palmitic acid	2.3	[9]
Stearic acid	2.51	[9]

D.2.2: n-Alkanes and iso-Alkanes for SAF Property Calculations

Table 2: Properties of alkanes used in ASTM property calculation for the SAF produced in Mannion model.

Molecule		Freezing point	Density	Flash Point	Net heat of Combustion	Viscosity	DCN	Final boiling point	Surface Tension
Chain Length	Name	C	kg m-3	C	MJ/kg	mm ² /s		C	mN/m
C-9	Nonane	-53 [21]	717.6 [22]	31 [22]	-48.21 [23]	1.78 at -20 C [24]	60.9 [25]	150.47 [22]	22.85 [26]
C-10	Decane	-30 [21]	725.5 [22]	46 [22]	-48.10 [23]	2.61 at -20 C [24]	66.35 [25]	174.1 [22]	23.83 [26]
C-11	Undecane	-26 [21]	740.2 [22]	62 [22]	-48.00 [23]	3.61 at -20 C [24]	71.98 Mannion interpolation	195.9 [22]	24.66 [26]
C-12	Dodecane	-10 [21]	749.5 [22]	83 [22]	-47.92 [23]	3.774 at -10 C [24]	73.45 [25]	216.3 [22]	25.35 [26]
C-13	Tridecane	-5	756.4	94	-47.86	4.97 at -10 C	79.09	235.4	25.99

C-14	Tetradecane	[21]	[22]	[22]	[23]	[24]	Mannion interpolation	[22]	[26]
		6	762.8	100	-47.80	4.304 at 5 C	85.1	253.57	26.56
C-15	Pentadecane	[21]	[22]	[22]	[23]	[24]	[25]	[22]	[26]
		10	768.5	132	-47.75	5.54 at 5 C	90.74	270.6	27.07
		[21]	[22]	[27]	[23]	[24]	Mannion extrapolation	[22]	[26]

Table 3: Properties of iso-alkanes used in ASTM property calculation for the SAF produced in Mannion model. *The DCN properties for 2-methylnonane, 2-methylundecane, and 2-methyldodecane were not found, therefore the DCN of 2,6-dimethyloctane, 3-ethyloctane, and 2,5-dimethylundecane were used instead. The Mannion average for the other iso-alkanes are the average of these DCN values.

Molecule		Freezing point	Density	Flash Point	Net heat of Combustion	Viscosity	DCN	Final boiling point	Surface Tension
Chain Length	Name	C	kg m ⁻³	C	MJ/kg	mm ² /s		C	mN/m
C-9	2-methyl-octane	-80.1	713	26	-47.76	-	52.6	143.2	21.88
C-10	2-methyl-nonane	[21]	[28]	[29]	[23]		Mannion average	[22]	[26]
		-74.6	728	46	-47.58	-	51.7*	166	-
		[21]	[28]	[30]	[23]		[25]	[30]	
C-11	2-methyl-decane	-48.9	737	50.1	-	-	52.6	189.3	-
C-12	2-methyl-undecane	[21]	[28]	[31]			Mannion average	[22]	
		-47	745.8	42	-	-	48*	195	-
		[21]	[28]	[32]			[25]	[32]	

C-13	2-methyl-do decane	-26	754	70.6	-	-	58*	227	-
		[21]	[28]	[22]			[25]	[22]	
C-14	2-methyl-tri decane	-25	761	79.5	-	-	52.6	245.2	-
		[21]	[22]	[33]			Mannion average	[33]	
C-15	2-methyl-tet radecane	-8	766	87.7	-	-	52.6	261	-
		[21]	[22]	[34]			Mannion average	[22]	

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