Title, Authors, and Affiliations

Life cycle assessment fuel production emissions of used cooking oil derived hydroprocessed renewable jet sustainable aviation fuel by a mass and energy balance

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Highlights

- Virtual biorefinery simulates changes in production for emissions reduction.
- A clear GHG emissions analysis for each step in production is presented.
- This model is validated against other tools and gives ASTM certified SAF.
- Clean electricity and green hydrogen shows decrease in production emissions.
- This model uses more representative and realistic inputs than current LCA tools.

Graphical Abstract
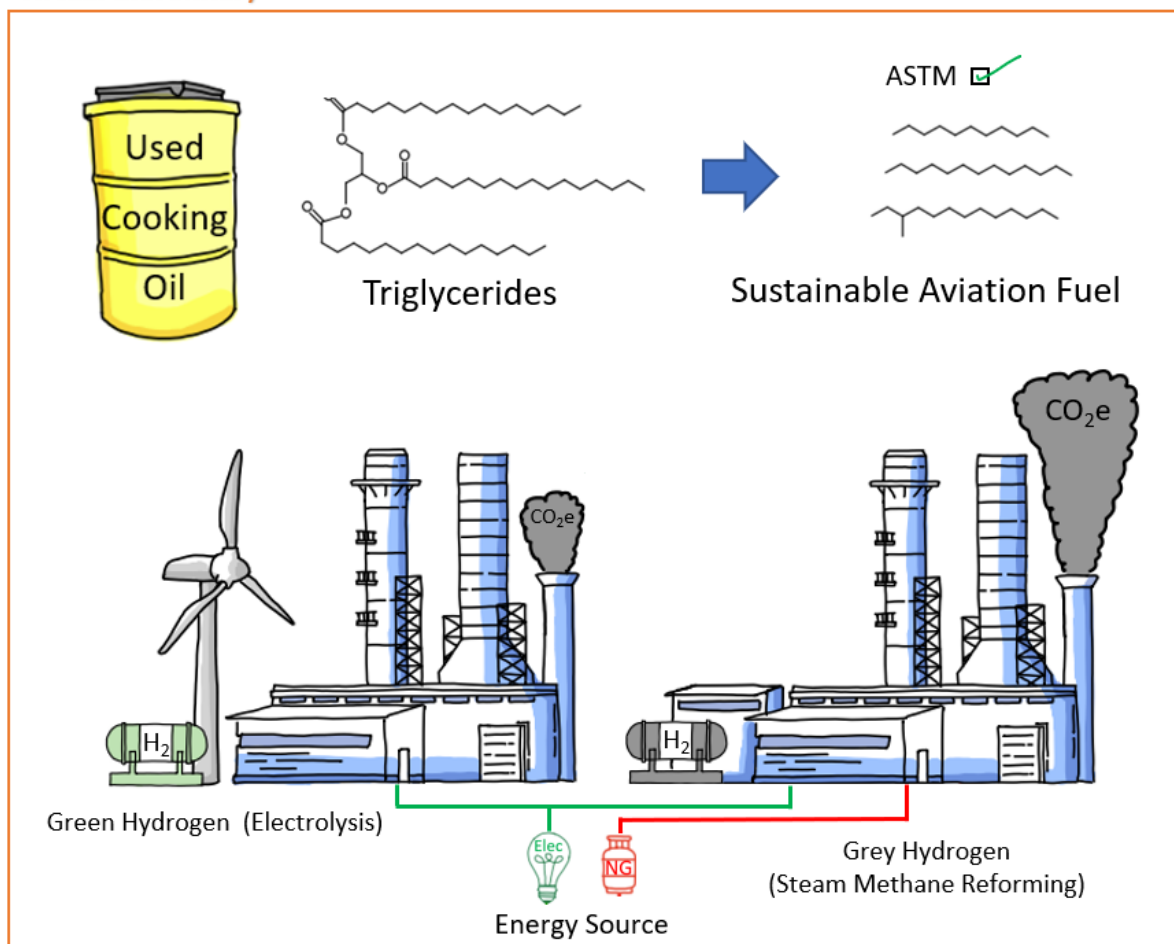
Life cycle assessment fuel production emissions of used cooking oil derived hydroprocessed renewable jet sustainable aviation fuel by a mass and energy balance

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Abstract

This paper uses a mass balance and reaction mechanistic approach to determine the lifecycle fuel production emissions of used cooking oil derived hydroprocessed renewable jet (HRJ[1]) sustainable aviation fuel (SAF[2]). A model is built using the described methodology providing a breakdown of emissions for each production step, hydrogen use, and intrinsic CO_2 produced, expressed in gCO_2e/MJ_{SAF}[3]. The transparency of the model allows for a virtual representation of any vegetable oil based biorefinery based on triglyceride composition, creating a comprehensive analysis of their production emissions, and opportunity for optimization. Current open-source life cycle assessment (LCA[4]) calculators are not capable of this. Analysis shows that while it is verified by existing LCA tools, the data used in this work is more agreeable with current experimental literature. This, paired with the advantage of this model to see the individual greenhouse gas intensity contribution for each step in production creates a more descriptive and representative LCA model for current physical biorefineries fuel production emissions. By using this model to simulate changes in production, energy and material cost can be reduced, decreasing the embodied emissions of the SAF. A scenario analysis shows production emissions can be greatly reduced using clean energy and green hydrogen. Furthermore, the effect of co-product allocation method is discussed. The mass-based reaction mechanism gives individual proportions of n-alkanes and iso-alkanes in the range of C-9 to C-15 which allowing for a property analysis of the HRJ SAF produced by the model which agrees with ASTM[5] D1655/ D7566 standards.

Keywords: Life cycle assessment, sustainable aviation fuel, used cooking oil, greenhouse gas emissions reduction, bio-jet fuel, mass balance.

1. Introduction

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[1] Hydroprocessed renewable jet, a type of sustainable aviation fuel.
[2] Sustainable Aviation Fuel.
[3] Unit of life cycle assessment, grams of carbon dioxide equivalent per mega joules of the produced sustainable aviation fuel.
[4] Life cycle assessment, the calculation of embodied emissions associated with renewable fuels use.
[5] American Society for Testing and Materials, international standard organisation for jet aviation and synthetic aviation fuel.

In 2017, aviation represented 2% of all global anthropogenic CO_2 emissions [1]. Petroleum derived Jet-A fuel is the leading contributor of these emissions. In 2009, the United States consumed 99.8 EJ of energy, with around 40% of this energy derived from petroleum. Under CORSIA, petroleum based Jet-A releases 89 gCO_2e/MJ of fuel burned [2], this is a substantial amount of carbon dioxide equivalent that can be reduced with the use of SAF [3]. SAF produced from waste feedstocks or renewable sources is a promising low carbon fuel that is widely considered as a medium-term solution for reducing aviation emissions [4]. Fuel production and feedstock cultivation are considered the largest contributors to total LCA emissions for sustainable aviation fuel production [5]. When working with waste products however, the cultivation element of the feedstock is not considered in the LCA calculation [6]. Hence the largest contributor of greenhouse gas emissions from sustainable aviation fuel produced from waste materials is fuel production [7].

Life cycle assessment (LCA) is needed to compare the emissions of petroleum-based fuel to the total embodied emissions in producing synthesised fuel. When considering the emissions from petroleum-based fuel we consider only the combustion of the fuel itself, while with synthesised fuels the combustion element is net carbon zero [8]. When producing biofuels and renewable fuels however, the life cycle emissions from feedstock cultivation, harvesting, feedstock transportation, fuel production, fuel transportation and distribution, and other areas need to be considered [8]. This is known as the "Well-to-Wake" is the emissions of the finished fuel [9, 10]. The unit to measure these emissions is generally gCO_2e/MJ, where 'e' denotes 'equivalent' [11]. This contains non-CO_2 emissions such as NO_x or CH_4 that are formed alongside CO_2 during the Well-to-Wake process, which are converted to CO_2e by the IPCC global warming potential guidelines [12]. The total Well-to-Wake emissions of the produced sustainable aviation fuel is variable depending on feedstock used, transportation routes, fuel production methods, location of facilities, LCA methodology used, and many other factors [13]. This highlights the need of LCA tools.

Life cycle assessment tools are calculators that provide the total Well-to-Wake emissions of various bio-based fuels. The Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model (GREET) [14], GHGenius [15], and BioGrace [16] are some of the most prominent LCA tools in literature used quantify embodied emissions of sustainable aviation fuel [17]. They are open source and free to use, providing the perfect comparison for research in LCA [17-19]. These tools are excellent for performing full Well-to-Wake LCA calculations, however, when isolating individual LCA areas, the detail in the models is lacking. In some cases, the tools can be modified or altered to determine the effect of changing on LCA area [20], while in other cases the tools need to be completely modified [7]. For hydroprocessed renewable jet fuel well-to-wake calculations in LCA tools, fuel production is represented by a limited set of default inputs and data, with the most commonly declared inputs in literature being hydrogen production parameters and total energy use [7, 21, 22]. The simplistic inputs within these models does not allow for further elaboration of possible

areas in fuel production emissions. In GREET, GHGenius, and BioGrace, the hydrogen use and total energy use have default values depending on the SAF production pathway and feedstock used. Our knowledge of the calculation behind these values is limited, as the input is unreferenced, and accuracy unknown.

This is an area in LCA that can be further investigated. By modelling a virtual biorefinery is possible to elaborate on the specific areas that contribute to the total fuel production emissions. The model created in this work uses a mass balance and reaction mechanistic approach to estimate the greenhouse gas intensity in the conversion of used cooking oil to hydroprocessed renewable jet sustainable aviation fuel. This approach can be used to accurately determine the individual energy use of each production step, while also counting how much hydrogen is needed for conversion. The model uses the physical properties of the molecules present in the feedstock to determine this. The output of the model shows the individual greenhouse gas intensity contribution of each processing step, hydrogen use, and intrinsic CO_2 produced during conversion of feedstock to fuel. This model can therefore be used by fuel production facilities to simulate changes in their biorefinery that would reduce their greenhouse gas emissions. The model can be customised and adapted to incorporate renewable hydrogen use, renewable electricity production, and assess other vegetable oil feedstocks.

This paper focuses on the fuel production element of life cycle assessment. The aim of this study is to quantify the total gCO_2e/MJ_{SAF} of used cooking oil derived hydroprocessed renewable jet sustainable aviation fuel by creation of a mass and energy balance trough a triglyceride reaction mechanism. The system boundary of this LCA study is shown in Figure 1. It shows the elements of fuel production considered in this work. This model was derived completely from first principles, using the most up to date academic literature in this area. By creating this virtual biorefinery, it is possible to estimate the greenhouse gas intensity (gCO_2e/MJ_{SAF}) of each of the production areas defined in Figure 1 and use the model to see how the greenhouse gas intensity can be reduced in these specific areas. This work provides a clear, transparent methodology in calculating the fuel production emissions of sustainable aviation fuel. It provides a model that isolates the GHG intensity of different areas of production, allowing for fuel production facilities to simulate changes in their fuel production facility to minimise their emissions. Therefore, this model can be used to optimise the fuel production process of any hydroprocessed renewable jet fuel biorefinery.
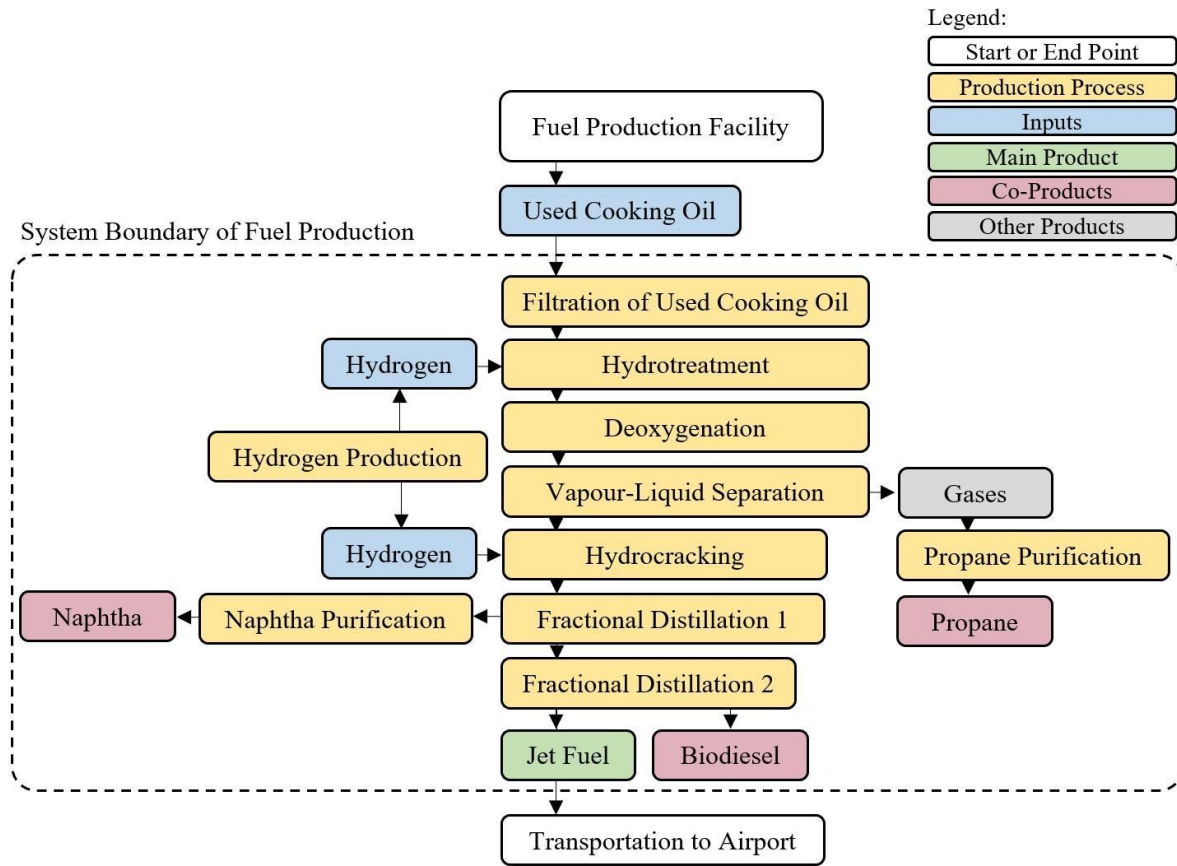
Figure 1: System boundary of fuel production emissions. Arrows dictate the flow of mass through the fuel production system. Elements within the rounded rectangle are considered and modelled in this LCA study, while elements outside are not considered.

2. Methodology

2.1. System Boundary

The sustainable aviation fuel is produced through the hydrogenation of vegetable oil (HVO) from waste products, and in this case is 100% used cooking oil. The SAF is therefore hydrotreated renewable jet (HRJ) aviation fuel. The system boundary is described in Figure 1, defined through examination of academic literature [23-26]. The system boundary begins with the filtration of the used cooking oil and ends with the ASTM certified hydrotreated renewable jet fuel, ready for transportation to the airport, or blending facility. The assumptions for each processing step are listed in Appendix A.1.

2.2. Mass and Energy Balance

To determine the total emissions associated with fuel production, a mass and energy balance for each processing step was constructed. The aim of this mass and energy balance is to quantify the energy use, hydrogen use, and intrinsic CO_2 production in conversion of used cooking oil to hydroprocessed renewable jet fuel. The model follows the flow of mass from 100 kg of used cooking oil feedstocks through the processing steps in Figure 1 and observing the molecular changes through the reaction

mechanism described in Section 2.3. From this, the energy required for these molecular changes can be estimated using the physical properties of the molecules, while calculating the hydrogen needed for conversion and the CO_2 produced through balanced chemical equations in the reaction mechanism, referred to in this paper as intrinsic CO_2.

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

$$E_{Total} = E_{Filtration} + E_{Initial\ Hydrotreatment} + E_{Propane\ Cleave} + E_{Deoxygenation} + E_{Vapor-Liquid\ Separation} + E_{Second\ Hydro}$$

$$\#(Equation\ 1)$$

For example, during filtration the used cooking oil is heated from 25 C to 35 C for mesh filtration and is then heated to 100 C to remove water. The specific heat capacity of triolein, tripalmitin, and trilinolein are used to find the energy required for this processing step, shown in Equation 2.

$$E_{Filtration} = m_{Triolein} C_{p_{Triolein}} (75\,°C) + m_{Trilinolein} C_{p_{Trilinolein}} (75\,°C)$$

$$+ m_{Tripalmitin} C_{p_{Trialmitin}} (75\,°C) + m_{Unknowns} C_{p_{Unknowns}} (75\,°C)$$

$$\#(Equation\ 2)$$

Where m is the mass and C_p is the specific heat capacity of each molecule listed. The unknowns in Equation 2 account for the molecules in used cooking oil that are non-triglycerides. These molecules are a mixture of diglycerides, monoglycerides, and free fatty acids. Here, the average of the specific heat capacity of these molecules is used. Initial hydrotreatment, deoxidation, second hydrotreatment, and fractional distillation 1 and 2 are processes that require heat energy. Other processing steps require inputs for specific cases, such as vapor-liquid separation, and naphtha purification. For a detailed breakdown of each term in Equation 1, see Appendix B.1.

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

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

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. It is assumed that the used cooking oil is heated to 420 C and maintained at 33% efficiency, and this low efficiency accounts for the energy that would be required to keep the fuel mixture at constant temperature.

The total energy use is then split between four areas of possible energy generation: electricity, diesel/gasoline, natural gas, and coal. The emission factors for each of the fuels are from literature sources [12, 27]. The default model assumption sets the energy use to 100% electricity, as the

electricity grid greenhouse gas intensity is representative of clean energy standards are in different countries. The fuel production facility was chosen to be Finland as there are various upgrading facilities in Finland that produce used cooking oil derived hydroprocessed renewable jet sustainable aviation fuel and provides this SAF across Europe.

2.3. Reaction Mechanism

Used cooking oil can be represented as proportions of triglycerides, diglycerides, monoglycerides, and free fatty acids [28]. This work uses a reaction mechanism that describes the conversion of triglycerides to free fatty acids, and free fatty acids to long chain alkanes. The three triglycerides chosen are triolein, tripalmitin, and trilinolein, as these triglycerides are hydrotreated to form palmitic, stearic, oleic, and linoleic acid. These free fatty acids are 99.3% representative of the chosen sunflower oil based used cooking oil [24]. Sottelo-Boyás et al, Tao et al., Barbera et al., and Scaldaferri et al. [24, 29-31] were used to create this reaction mechanism. Figure 2 shows the reaction mechanism for triolein, displaying a summarised reaction pathway that is one part of the full reaction mechanism found in Appendix C.1.
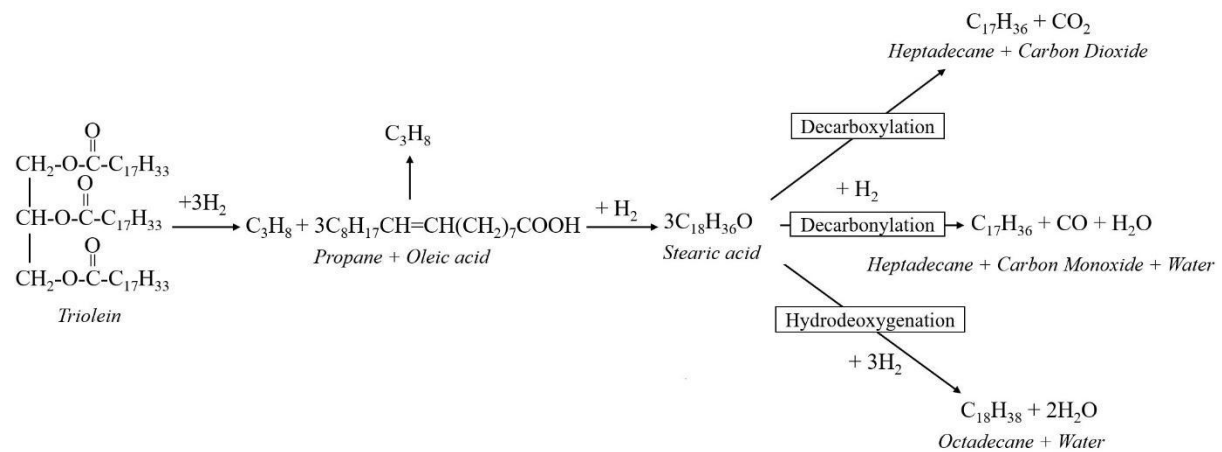

Figure 2: Summarized triglyceride reaction mechanism. Triolein to heptadecane, octadecane, carbon monoxide, carbon dioxide, and water in the presence of hydrogen under high temperature conditions.

The triglycerides are hydrogenated to free fatty acids, forming propane in the process [24]. The fatty acids undergo deoxygenation in three separate processes: decarboxylation, the removal of oxygen in the form of CO_2, decarbonylation, the removal of oxygen by the formation of carbon monoxide and water, and hydrodeoxygenation, the removal of oxygen by the formation of water [31]. The use of a catalyst can affect the proportions of free fatty acid decarbonisation pathway leading to different proportions of gas formed as a result of conversion, this can impact the greenhouse gas intensity of the fuel [32]. This is discussed in Appendix C.2. This work uses a NiMol catalyst, and therefore it is assumed that the free fatty acids follow the decarbonization pathway of 68% decarboxylation, 3% decarbonylation, and 29% hydrodeoxygenation (mass%) as outlined in Chu et al. [33]. The products of the reaction mechanism are leftover hydrogen, water, carbon monoxide, carbon dioxide, propane

(C-3), n-alkanes (C-15 to C-18), and n-alkenes (C-17 to C-18). It is then assumed that the n-alkenes are saturated to n-alkanes. The n-alkanes must then be cracked to give the required carbon range of HRJ.

2.4. Hydrocracking

The reaction mechanism concludes with a mixture of n-alkanes and ranging in carbon length C-15 to C-18 [24]. The fuel mix is then hydrocracked under conditions of 420°C, 1 h^{-1} LHSV, at 10 MPa, and 2200 H_2/oil ratio [34]. The C-15, C-16, C-17, and C-18 alkanes are cracked to produce a range of alkanes from C-4 to C-18. This results in a distribution of 56.8% Jet Fuel (C-9 to C-15), 35.3% Naphtha (C-4 to C-8), and 7.8% Diesel (C-17 to C-18), at 100% conversion rate. Verma et al. describes this cracking methodology experimentally [34], which is used in our analysis to provide an accurate description of current hydrocracking technology. In the mass balance, Naphtha contains the n-alkanes that would conventionally be attributed to LPG (C-4 to C-5), this does not affect the LCA mass or energy allocation emissions. The mass balance determines how the long chain n-alkanes split in the fuel mix. Here, a GCxGC analysis of a HEFA surrogate [35] was chosen to validate alkane hydrocracking assumptions, while complying to the yield limitations and iso-alkane conditions defined in Verma et al [34]. It is assumed that the alkanes are isomerised to a mixture of 17% C-n, and 83% 2-methyl-(n-1).

2.5. Hydrogen and CO_2 Accounting

The mass of hydrogen used, and intrinsic CO_2 formed are calculated using the balanced chemical equations from the model, shown in SIX.X, and observing the flow in mass through the reaction mechanism. By knowing the input mass of the triglycerides, it is possible to calculate the mass of hydrogen used and CO_2 produced during conversion. For determining hydrogen use during cracking, the alkane chemical structure was used to quantify the hydrogen needed to saturate broken bonds, for example, when C-18 cracks to C-10 and C-8, two H atoms are required for saturation to C-8 and C-10 alkanes.

2.6. Conversion to gCO$_2$e/MJ$_{SAF}$

The net energy use in fuel production, E_{Net} (J), is then converted to gCO$_2$e/MJ$_{SAF}$. The unit gCO$_2$e/MJ$_{SAF}$ is the standard value used in SAF LCA and is defined as the total gCO$_2$e per MJ of SAF produced. The definition of E_{Net} (J) is the energy required to convert 100 kg of used cooking oil to SAF and co-products. Therefore, we need to consider the yield (kg SAF/ kg used cooking oil), and the lower heating value (MJ/kg), or energy density of the produced SAF. This conversion is also performed for the hydrogen use, and the intrinsic CO_2 cost in SAF production, determined by a mass balance of the reaction mechanism in Figure 2. The equation for these conversions is shown in Appendix B.2.

The total production emissions are the summation of the three areas of energy use, hydrogen use, and intrinsic CO_2 formed. Energy, mass, and displacement allocation methods are then applied to the calculated value to give the final LCA greenhouse gas emissions in gCO_2e/MJ_{SAF}. Further information on allocation method calculations is contained in Appendix B.3.

3. Results and Discussion

3.1. Comparison to LCA tools and Literature

Figure 3 displays the calculated fuel production emissions of this work to the default production emissions of used cooking oil derived hydroprocessed renewable jet fuel from LCA tools GHGenius, and BioGrace, Seber et al.'s modified GREET, and further compared with literature and policy values. GHGenius and BioGrace are within 17% and 26% respectively of this work's value, while Seber et al.'s GREET [7], Capaz [6], De Jong [5], and CORSIA [36] disagree by 21%, 20%, 87%, and 17% respectively.
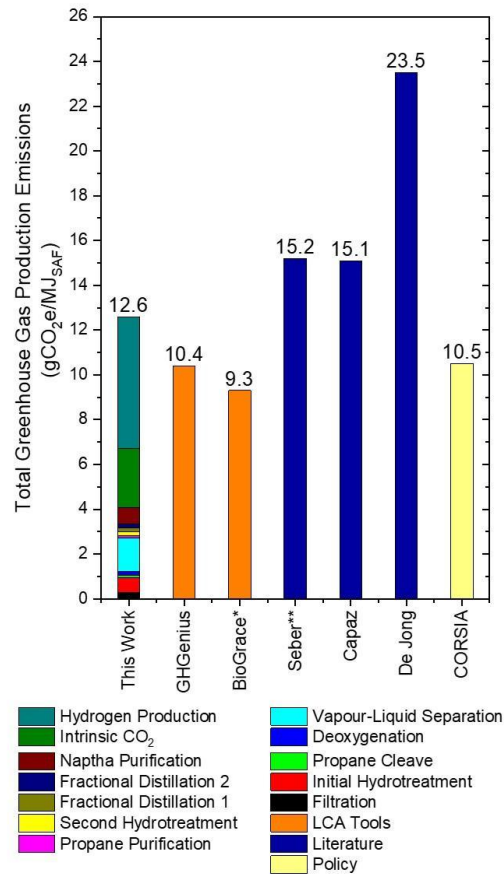

Figure 3: Results of used cooking oil derived hydroprocessed renewable jet fuel production emissions. This works model with energy allocation is compared to default fuel production emissions of GREET, GHGenius, BioGrace, literature studies, and policy values. *BioGrace production emissions were calculated by modelling the HVO production emissions of sunflower oil. BioGrace cannot model used cooking oil, however the production process for sunflower oil HVO is identical to used cooking oil HRJ other than filtration. **Seber et al.'s paper [7] was used for the GREET Model values. Seber et al. uses a modified GREET version, as GREET cannot model used cooking oil for SAF production, therefore it is under literature.

Seber et al. [7] uses a modified GREET model for its LCA study, and Capaz et al. [6] used some of the same inputs as observed in Seber et al. [7], leading to almost identical production emissions. The inputs within GREET are not completely representative of used cooking oil conversion to hydroprocessed renewable jet fuel, as GREET cannot yet model this. De Jong [5] also uses default GREET values for some production parameters. The default energy use in GREET split between electricity and fossil fuels, with the main form of energy production being natural gas. However, in this work, the default model assumptions, the only energy source is from electricity. The greenhouse gas intensity of clean electricity used in this work gives a much less carbon cost to energy use, which is the reason for the discrepancy compared to Seber, Capaz, and De Jong. However, this work's model can incorporate natural gas energy use. To observe this, see Scenario 1 and Scenario 2 in Figure 4, where the production emissions value is in more agreement with these literature. CORSIA shows a 17% difference in production emissions. CORSIA states to use the modified GREET Seber et al. tool [36]. There are noticeable differences between the Seber et al. GREET value and the CORSIA value, which shows the wide variability when using the same tool for emissions analysis. This is a benefit the model described in this work has, as it is easier to determine discrepancies within the model due to the individual areas of emission sources being reported and visualised. The level of detail in the model allows this.

The analysis of literature and policy values show that the same generic input values are being used for the production emissions analysis of used cooking oil derived hydroprocessed renewable jet fuel. This is a display of the lack of research in this area. This work creates more inputs in this area of life cycle assessment, while using data more representative of actual fuel production parameters to calculate the fuel production emissions (see Figure 4). As well as this, the model methodology is discussed with clear transparency, while allowing the user to observe the individual greenhouse gas intensity in different production areas. This unique, clear methodology therefore has the potential to be used by actual biorefineries and optimise their production process while reducing emissions.

3.2. GHGenius and BioGrace Discrepancy
3.2.1. Hydrogen Emissions

GHGenius and BioGrace are open source LCA tools. While GHGenius is updated yearly [REF}, BioGrace is a slightly outdated, still using the RED I methodology {REF Website]. BioGrace also models pure vegetable oil rather than used cooking oil, therefore production parameters like filtration are not considered. The discrepancy between these the tools and this work is however the hydrogen production parameters, energy use in conversion, and intrinsic CO_2 formed.

Table 1 shows the hydrogen production parameters within GHGenius and BioGrace tools compared to this work. GREET could not be investigated as it cannot currently model used cooking oil SAF. The difference in parameters arises in the emission factor for hydrogen production. GHGenius assumes a

12.17 kg CO_2 released per kg of H_2 used, while BioGrace assumes 10.5 kg CO_2 /kg H_2. Therefore, even though all models estimate a similar use of hydrogen in conversion, this leads to differences in total GHG intensity. The emission factor of hydrogen production used in this work is a 2022 calculation of the life cycle assessment of steam methane reforming of natural gas [37]. For model verification, the production parameters of GHGenius were used in the model described in this work. When this works model uses GHGenius hydrogen production parameters, there is a maximum deviation of 6%. This small deviation provides credibility to this works hydrogen calculations, as it is consistent with GHGenius in this area. This is discussed further in section X.X.

Table 1: Hydrogen Production Parameters and emissions comparison of this work to GHGenius and BioGrace. Each value declared is a parameter used in calculating the total emissions attributed to hydrogen use in the total production emissions of used cooking oil derived hydroprocessed renewable jet fuel.

Tool	Hydrogen use (kg H_2/kg HRJ)	Hydrogen Emission Factor (kgCO_2/kg H_2)	Yield of HRJ from 100% feedstock	HRJ LHV (MJ/kg HRJ)	Unallocated Hydrogen Production Emissions (gCO_2e/MJ)	Allocation of co-products (gCO_2e/MJ)	Allocated Hydrogen Production Emissions (gCO_2e/MJ)
This work	0.056	8.47	0.48	43.74	10.98	-5.11	5.87
GHGenius	0.057	12.17	0.70	44.10	16.01	-5.58	10.39
BioGrace	0.044	10.50	0.97	44.00	10.50	-1.09	9.41

3.2.2. Comparison with Literature

Figure 4 shows a comparison of some of the parameters used, or derived, in this work, compared to literature and LCA tools GHGenius, BioGrace, and GREET. Figure 4 (a) shows the yield of used cooking oil derived SAF from experimental literature, LCA tools, and this work. The green symbol shows the average and standard deviation of the literature and LCA tool values. The blue symbol shows the value used in this work.

Figure 4 (a) shows that current LCA tools generally fall outside the range of one standard deviation of the mean, while this work gives a yield that is more accurate to experimental data. This indicates the declared SAF yield in current LCA tools is not consistent with literature.

Figure 4 (b) shows the same comparison for hydrogen use. This reveals how much hydrogen is required to make 1 kg of SAF. Depending on the assumptions in the model, this value can vary [30]. This value is expressed as hydrogen used per HRJ produced. Barbera et al compares the hydrogen use per kg of used cooking oil used, and found from literature that the hydrogen used is generally in the range of 2-4% [30]. This study agrees with this range, at 2.7%. Expressing hydrogen use in terms of HRJ produced takes the yield of HRJ into account, this allows for better comparison of the models. In an ideal case, the hydrogen use per kg HRJ produced should conform to a defined range, if the

reaction conditions are similar. This is what is observed in Figure 4 (b), with the exception of Pearlson et al. [38]. Figure 4 (b) shows that the modelling performed in this work agrees with current LCA tools and most literature values within one standard deviation. This analysis therefore verifies this works hydrogen use parameters, as it agrees with current LCA tools, and literature.

Figure 4 (c) shows the range in hydrogen emissions share (% of H_2 production emissions of total production emissions). The range in total production emissions due to hydrogen is from 44-100%. Some tools consider mostly or only emissions relating to hydrogen in the total production emissions of SAF, with some agreement in the literature [6]. This work considers many areas of fuel production emissions, which decreases the total share of emissions from hydrogen alone, this is consistent with Barbera et al. [30] and De Jong et al. [5]. For this work, the methodology behind total fuel production emissions is transparent and shows clearly where emissions arise. Where literature studies do not completely rely on LCA tools, it is observed that hydrogen emission share is lower, in agreement with this work [5, 30].
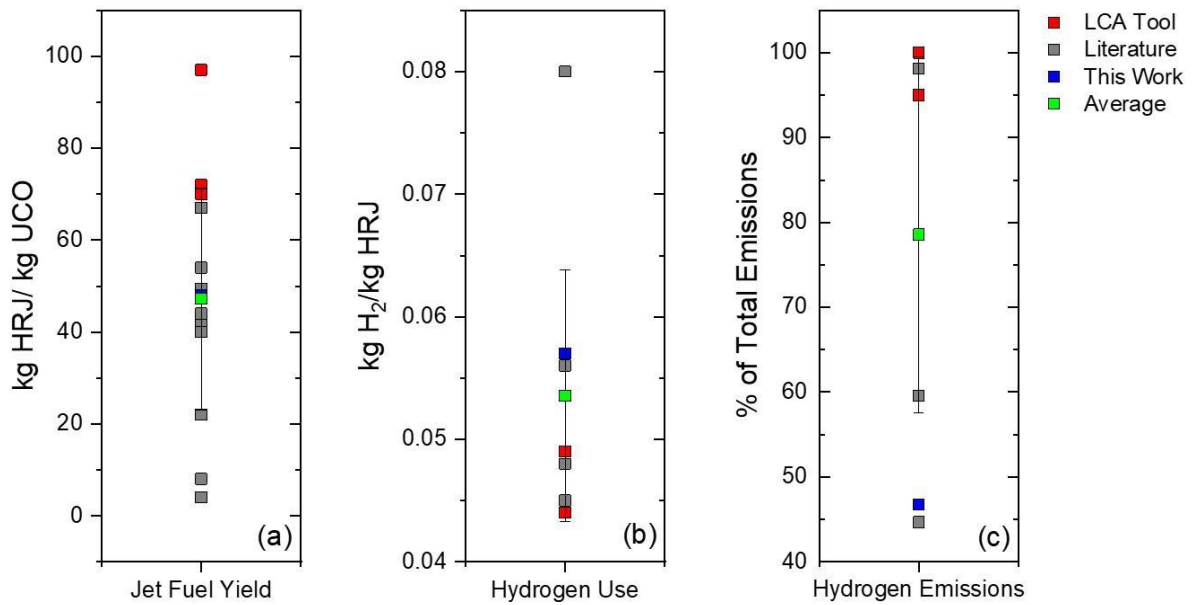

Figure 4: Comparison of this work's inputs and derived values compared to existing LCA tools and literature values, for the areas of Jet Fuel Yield (a) [7, 14-16, 29, 30, 34, 39], Hydrogen Use (b) [14, 16, 30, 33, 38], and Hydrogen Emissions Share (c) [5, 6, 30].

3.3. Scenario Analysis

Figure 4 displays the effect on the overall LCA value from the use of green hydrogen and electricity use in four separate scenarios using the model described in this paper. Scenario 1 is the fossil fuel scenario, using 90% natural gas and 10% electricity as an energy source, using grey hydrogen from the steam methane reforming (SMR) of natural gas. Scenario 2 is the default scenario in the fuel production model, it uses 100% electricity as an energy source, and grey hydrogen. Scenario 3 uses

90% natural gas and 10% electricity as an energy source, using green hydrogen from the electrolysis of water using renewable energy. Scenario 4 is the green scenario, using 100% electricity as an energy source and green hydrogen. Figure 4 shows there is a sharp decrease in the production emissions of hydroprocessed renewable jet fuel when clean electricity and green hydrogen are used. This work assumes the production plant is in Finland. Finland is known for clean and renewable electricity, with a average electric grid emission factor of 21.39 gCO_2e/MJ [27]. When this is paired with the low emission factor of green hydrogen (1.57 kg CO_2e/kg H_2) [40] instead of the widely commercial grey hydrogen from steam methane reforming of natural gas (8.47 kg CO_2e/kg H_2) [37], a significant amount of CO_2e can be saved.
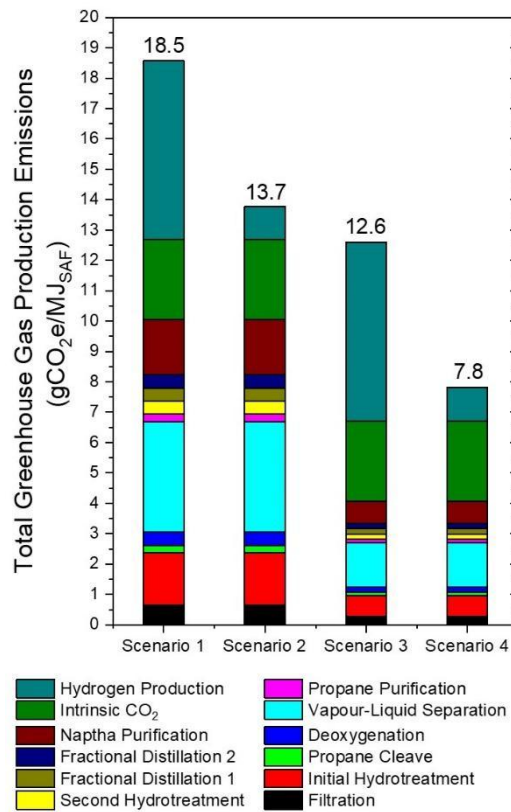

Figure 5: This work's production emissions using different production parameters. "Grey" denotes the use of grey hydrogen, produced from steam methane reforming (SMR) of natural gas. "Green" denotes the use of green hydrogen, produced by electrolysis from renewable wind electricity. "Electricity" denotes the use of 100% electricity as an energy source. "NG" denotes the use of 80% natural gas and 20% electricity as an energy source.

3.4. Co-Product Allocation Deviations

Co-product allocation methods can greatly influence the overall LCA value. Figure 4 shows the difference in LCA value for mass, energy, and displacement allocation methods. Energy allocation takes the total greenhouse gas intensity of production and allocates it by how much SAF energy (MJ) is present in the total combustible products formed. For this, the energy density of the fuel, and masses of SAF and co-products formed is required. Mass based allocation is similar, it allocates

emissions by total percentage mass in the main product and co-products formed. Displacement uses the masses of co-products formed and calculates an emissions savings of replacing the fossil fuel versions with the bio-alternatives formed in production. Using displacement allocation, it is possible to significantly reduce the greenhouse gas intensity of production as However, this is not completely representative of the actual emissions involved in SAF production. Displacement is an ambitious form of co-product allocation; it takes all the emissions savings from each of the bio-co-products and applies it to one product. This isn't practical as the use of these co-products would therefore offer little to no emissions savings to the user because they are already accounted for in the SAF. This limitation is observed in Ukaew et al. [41], and discussed in Han et al. [21], where they discuss how the displacement method may not be an acceptable allocation method when the share of co-products is high. Therefore, energy and mass allocation are a much more practical allocation method, as the total LCA value is divided among both the main and co-products. This promotes the use of each product formed in HRJ production, as each co-product has an allocated LCA value, allowing for emissions savings in other industries, and therefore higher revenue streams for the production plant.
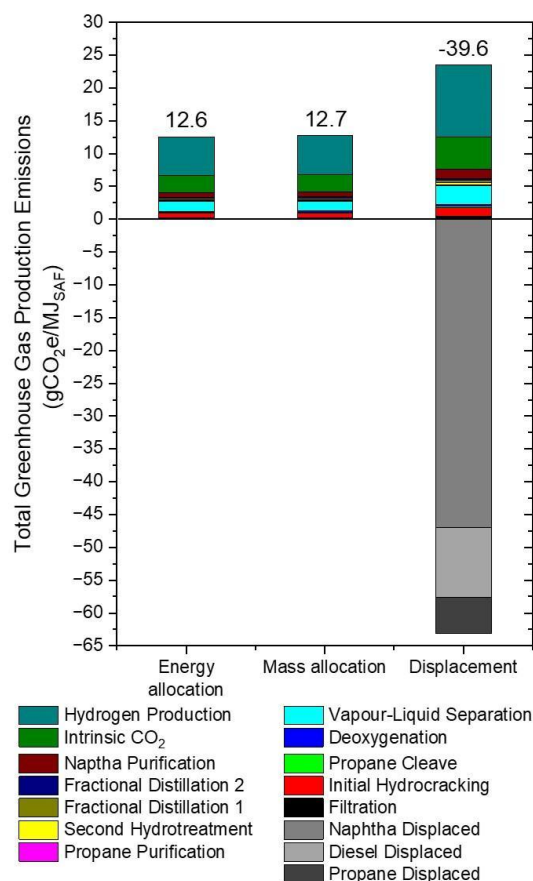

Figure 6: Co-product allocation methods visualised. Energy, mass, and displacement allocation methods applied to the mass and energy balance results in this work's fuel production model.

3.5. Mass Balance Result

Each co-product allocation method is dependent on the masses of co-products formed in HRJ production. This implies there must be accuracy in the mass balance to obtain a representative greenhouse gas intensity value. The mass balance presented uses the most up to date literature values that experimentally describe the refuel production process.

Table 2 shows the result of the mass balance in this work's fuel production model. Out of x studies discussed in this paper, 3 of x produced a table of total products of the reaction mechanism as shown in Table 2. Table 2 shows the end products of the reaction mechanism described in Figure 2. By following the flow of mass from triglycerides to straight chain alkanes, it is possible to accurately quantify these products. The benefits of this analysis is a quantitative and qualitative analysis of the hydrogen use, and products formed as a result in creating HRJ fuel. This allows for an analysis of intrinsic CO2 formed as a direct result of converson. This is something that isn't considered in most life cycle assessments. For example, Seber et al [7] uses direct data from Pearlson et al.'s [38] mass and energy balance for conversion of soybean oil to HRJ, but does not mention the cost of producing this CO_2 in their life cycle assessment. Rather, Seber et al. uses the energy use for conversion by use of natural gas or electricity to quantify the emissions associated with production. It is unknown if this intrinsic CO_2 evidenced in Pearslson's mass flow is accounted for here. In this work, we account for this, and show with transparency where it arises, and how it can be reduced. This table shows similar characteristics to the result of the mass balance in Pearlson et al.'s [38].

Table 2: Fuel production mass and energy balance results. Total mass adds to 110 kg as initial mass of used cooking oil is 100kg and hydrogen inputs total to 10 kg. Mass and energy are completely conserved.

Description	Unit	Value
Naphtha	kg	29.85
Jet Fuel	kg	48.02
Diesel	kg	6.62
Residual Oil	kg	0.00
Water	kg	6.53
Propane	kg	4.18
LPG	kg	0.00
Carbon Dioxide	kg	5.07
Carbon Monoxide	kg	3.23
Spare Hydrogen	kg	6.50
Total	kg	110.00
Jet Fuel Yield	% (kg SAF/ kg UCO)	48.02%

The distinct difference between the result in Table 2 and the result from Pearlson et al. [38] is the differences in renewable diesel and naphtha yield. This work shows 28% and 426% of Pearlson's diesel and naphtha yield respectively. This discrepancy mas minimal influence the fuel production

LCA calculation, as the primary concern is the jet fuel yield, which agrees within 3%. The discrepancy observed here is due to the higher temperatures used in the hydrocracking production step, leading to a greater yield in lower chain co-products [29, 34], like naphtha, and higher chain co-products, like diesel. This, paired with the Pearlson et al. mass balance representing the conversion of soybean oil rather than used cooking oil, gives reasoning for the differences observed in mass balances. Tao et al. [29] compares their co-product yield to Pearlson et al.'s mass balance. In their paper, they show a 72% yield of used cooking oil derived HRJ. When only main products and co-products are considered; propane, LPG, naphtha, diesel, and jet fuel, this can be compared to Pearlson et al.'s main product yield of 55%, and this works main product yield of 55%. The Tao et al. co-product yields show more similar results to this work, as their analysis is considered for used cooking oil. Overall, the first principles mass and energy balance described in this paper yield similar results to other mass and energy flows formed from industry-based software and literature, while providing a clear and transparent description to the individual areas that create embodied emissions.

There are some limitations in industry that are contained within this model. The most recent 2023 data on conversion of used cooking oil to hydroprocessed renewable jet fuel shows only a 55% yield of sustainable aviation fuel from pure alkanes [34]. This decreases when all products are considered, like in Table 2. A second limitation is the isolation of reaction pathways. It is possible to simulate a reduction of greenhouse gas intensity by isolating the decarbonylation reaction pathway. Emissions are reduced by using less hydrogen, and not producing CO_2, unlike the other pathways. This isolation can be done physically by the use of catalysts [32]. This concept is under constant investigation, as both the use of catalyst and the temperature of reactors can greatly influence the final product yield [32, 34]. If 100% of the free fatty acids react through the decarbonylation reaction pathway, the production emissions are reduced from 12.6 to 9.7 gCO_2e/MJ_{SAF}, using the default production parameters (Scenario 3). This is shown in more detail in Appendix C.2. Using a catalyst to push the reaction towards decarbonylation reactions therefore offer possibilities to further decrease the production emissions of the fuel.

3.6. ASTM Properties

The properties of the produced SAF can be estimated from the properties of the individual molecules determined from the mass balance. These properties are compared to the ASTM standards for alternative aviation fuel [24, 34, 42, 43]. Table 3 shows the properties of the SAF modelled in the mass flow is in accordance with the ASTM standards for alternative aviation fuels.

Table 3: Derived properties of SAF produced in this work. Method shows the standard ASTM method for this measurement. If a SAF falls outside the Limits shown, it is not suitable as a drop-in aviation fuel. Model Result shows the derived properties from analysis of the mass balance. The properties are calculated by a linear mass% mixing rule of n-alkanes and iso-alkanes properties. *This range of surface tension is temperature dependant from -10 °C to 40 °C, the result shown is calculated at 20 °C.

Properties	Unit	Method	Limits	Result
Freezing Point	°C	D 5972	-40 Jet A	-44.5
Density (at 15°C)	kg m^{-3}	D 4052	730-772	740.5
Flash Point	°C	D 3828F	38 (min)	55.9
Net heat of combustion	MJ/kg	D 4529	42.8 (min)	47.8
Aromatics	vol%	D 1319	8 - 25	0.0
Final boiling point	°C	D 86D	300 (max)	196.8
Acidity	Mg KOH g^{-1}	D 3242	0.015 (max)	0.0
Viscosity (at -20 °C)	mm^{2}s^{-1}	D 445	8 (max)	3.6
Sulphur	wt%	D 4294	0.30 (max)	0.0
DCN	-	D 6890	35-60	55.9
Surface Tension	mN/m	D 1331	22-29*	24.8

Table 3 shows that the HRJ SAF produced in this model are compliant with the ASTM D1655 [43] /D7566 [42] specifications. For a synthesised drop-in aviation fuel to be used, it must comply to the ASTM specifications shown above. The limits shown are a mixture of the D1655 and D7566 specifications. D1655 is the standard specification for aviation turbine fuels, and D7566 is the certification standard for civil aviation turbine fuels containing synthetic hydrocarbons. The table above shows the property limitations in these documents, compared to the pure properties of the SAF produced in the model.

The properties declared in Table 3 were calculated by a linear mass% mixture of the 17% n-alkanes and 83% iso-alkanes defined in the mass balance. The properties derived here are calculated using experimental data from Nist Webbook [44], Landolt-Börnstein [45-47], and others [48-50]. Where the iso-alkane properties could not be found, either properties of the n-alkanes or a similar iso-alkane was used. Aromatics and acidity show 0.0 vol% and 0 Mg KOH g^{-1} respectively. This is due to assumptions in the methodology that all free fatty acids are converted to n-alkanes, iso-alkanes, and co-product gasses only. For sulphur, the used cooking oil feedstock contains 0.0 wt% sulphur [28], therefore the final product is 0.0 wt% sulphur. The conventional DCN range for a hydroprocessed renewable jet fuel is within the range of 40-50 [35], and the boiling point is generally higher than in Table 3 [51, 52]. Only some iso-alkane properties for DCN were used. This is due to the limited data available for DCN measurements of pure components [48]. In this instance, some iso-alkane properties within the C-9 to C-15 range were used, and an average value was applied to some of the iso-alkanes to account for unknown values. This leads to a final DCN outside the conventional range, but within the range of the ASTM specifications. No aromatics or cycloalkanes are formed in the

reaction mechanism, leading to a low boiling point [53, 54]. Cycloalkanes generally have much higher boiling points than n-alkanes. As the mass balance does not contain any cycloalkanes, it is therefore expected for the derived boiling point to be lower than physically measured SAFs. However, the boiling point shown in Table 3 is still within the range of the ASTM specifications. The molecular distributions of the SAF and properties of the individual components used to calculate the values in Table 3 can be found in Appendix D.2.2. The properties above provide evidence of accuracy for the model described in this paper, showing the life cycle assessment fuel production emissions are those representatives of a real hydroproccessed renewable jet sustainable aviation fuel.

3.7. Model Validation

The HRJ SAF described in Section 3.6 is a product of the mass flow element in the model described in this work. This same mass balance provides energy and material calculations for the lifecycle production emissions. Analysing and verifying the properties of the mass derived SAF provides credibility to the model. This serves as model validation, as the mass balance used to provide emissions calculations produces a mass distribution of n-alkanes and iso-alkanes which give properties representative of an actual sustainable aviation fuel.

Figure 4 displays validation of the inputs and derived values from the model. Figure 4 (a) shows that the derived yield is consistent with current experimental literature. Figure 4 (b) shows the agreement of literature, LCA tools, and this work, with hydrogen use per kg of produced SAF. Since the hydrogen use is calculated by the mass flow, this acts as a secondary validation to the ASTM properties. Figure 4 (c) shows the shares of hydrogen emissions compared to the total emissions. While disagreeing with LCA tools, this work does agree with literature. There are not many detailed contributions to this area, and therefore a strong conclusion cannot me made here. However, this paper provides evidence that HRJ production emissions are more than just hydrogen use, and further adds to this gap in LCA.

For emissions analysis validation, GHGenius was used. Here, the parameters for GHGenius were inputted into the model described in this work. Since GHGenius considers hydrogen emissions as 95% of the production emissions, only the unallocated hydrogen emissions were used in both models as a comparison. This allows for both models to compare the same isolated values, while not letting the differences in model methodology to interfere. When the GHGenius SAF yield, hydrogen emission factor, and hydrogen use were inputted into this works model, the resulting emissions were 15.77 gCO2e/MJSAF, compared to GHGenius's 14.88 gCO2e/MJSAF. This is a 6% deviation from GHGenius. The reason for this deviation is due to GHGenious's hidden methodology calculations. When GHGenius's parameters are extracted, the resulting emissions due to hydrogen production alone total to 15.98 gCO2e/MJSAF using this work's methodology. Overall, this works LCA calculations

can replicate the literature prominent and widely used LCA model GHGenius's value to within 6% using the same parameters. This therefore validates the LCA calculations within this work's model.

4. Conclusion

The model described in this paper can be used to describe any virtual biorefinery. By studying this model, it is possible to provide a current description of the total production emissions in the conversion of used cooking oil to sustainable aviation fuel. However, information and collaboration from industry is needed to make this calculation more accurate, and representative to a specific biorefinery. Through optimization of the fuel production process and by integration of new technology, it is possible to reduce the embodied greenhouse gas intensity of the sustainable aviation fuel produced. This can be performed and shown by the use of this model, while providing a transparent description of the areas in production that attribute to the total life cycle assessment value of the fuel. Further reductions in greenhouse gas intensity can be observed using more sustainable and renewable energy and material sources. Showing that while the current default value of the model gives the production emissions to be 12.6 gCO_2e/MJ_{SAF}, it can be as low as 6.5 gCO_2e/MJ_{SAF}.

This work details the fuel production emissions of used cooking oil conversion to hydroprocessed renewable jet fuel. The results are expressed in the greenhouse gas intensity of each processing step, allowing for a comprehensive understanding of where the embodied emissions of fuel production emissions arise. This model can therefore be used by any biorefinery to analyse and optimise their production process and reduce the life cycle greenhouse gas intensity of their produced fuel. Fuel production emissions within current LCA tools are reliant on inputs that have an unclear calculation methodology. The methodology detailed in this paper describes a method of calculating these inputs with transparent science-based modelling, dependant on the physical properties of the feedstock and experimental literature data. Through detailed reaction mechanisms and mass and energy balances production, the energy use, hydrogen use, and intrinsic CO_2 production can be calculated and expressed in terms greenhouse gas intensity attributions from each step in production. The comparison of this works result compared to other LCA tools, literature, and policy values, shows the dependency of literature on recycled inputs for overall energy and hydrogen use. The methodology detailed in this paper shows how these inputs can be calculated by an analysis of the reaction mechanism involved in the actual conversion of used cooking oil to hydroprocessed renewable jet fuel and can be quantified using a mass and energy balance, while using real data from literature.

The scenario analysis of the production emissions shows the dependency of the greenhouse gas intensity on the source of energy and hydrogen. The analysis clearly shows how the embodied emissions of sustainable aviation fuel can be greatly reduced by providing a clean and renewable source of energy, and hydrogen. The scenario analysis shows there are still embodied emissions present in sustainable aviation fuel production when clean electricity and green hydrogen is used. This

is due to embodied emissions in green hydrogen production, such as transport and distribution, and the intrinsic CO_2 produced in the conversion of used cooking oil to hydroprocessed renewable jet fuel by decarboxylation reactions. This is an embodied emission that can be reduced by the use of carbon capture and storage (CCS) [37], however this is not considered in this analysis.

The model described in this paper is multi-use and can be used for various vegetable oil feedstocks, only requiring their composition in terms of triglycerides, diglycerides, and free fatty acids, and experimental data detailing the yields of SAF and co-products from the hydrocracking the vegetable oils. This model can be integrated into existing LCA tools to provide a more scientific approach to hydrogen use inputs rather than relying on external sources, and used by industry to obtain a transparent description of their emissions, while providing a tool for optimization.

Data Availability

Datasets related to this article can be found in the Appendix D.

Acknowledgements

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Appendix