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Life Cycle Assessment of Sustainable Aviation Fuel - Production Emissions of Used Cooking Oil Derived Hydroprocessed Renewable Jet

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A report submitted to the School of Physics for transfer to the Ph.D. register

Under the supervision of Dr. Stephen Dooley

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Abstract:

Life-cycle assessment (LCA) is used to determine the total upstream embodied emissions of renewable fuel use. In this project, TCD has developed a LCA model to quantify the total embodied emissions for specific Ryanair scenarios. This model is used to determine the total greenhouse gas (GHG) gCO_2e/MJ_{SAF} and gCO_2e/RPK emissions using real industry data and information from the actual feedstock producer, fuel supplier, airport logistic staff, and end users. The TCD LCA model is derived from first principles, rather than using existing LCA calculators. The TCD LCA model is divided into four sections: feedstock, fuel production, airport, and aircraft. The three sections: feedstock, fuel production, and airport, each contribute greenhouse gas emissions to the final LCA value in gCO_2e/MJ_{SAF}, which is converted to gCO_2e/RPK through the aircraft section of the TCD LCA model.

A description and discussion of the fuel production methodology is contained in this report. Other areas in the TCD LCA model are discussed elsewhere. Fuel production is the largest contributor to the total embodied emissions of the SAF, with emissions ranging from 15.14-24.05 gCO_2e/MJ_{SAF}. The conditioned TCD LCA value for fuel production is 15.31 gCO_2e/MJ_{SAF}, leading to a total TCD LCA value of 23.23 gCO_2e/MJ_{SAF} for hydrotreated renewable jet fuel (HRJ) from used cooking oil (UCO) feedstock sourced from Indonesia. This calculated value shows nearly triple the LCA value than Neste's claimed LCA greenhouse gas emissions (7.51 gCO_2e/MJ_{SAF}), and nearly double the LCA value than CORSIA's default core value (13.9 gCO_2e/MJ) for the same conditions.

Ryanair Scenario 1 was defined and analysed in these four areas. It was found that the use of Neste SAF in Ryanair's Boeing 737-8200 MAX from Amsterdam Schiphol Airport to Dublin Airport yielded a LCA range of 16.56-24.85 gCO_2e/MJ_{SAF} or 12.97-18.17 $gCO2e/RPK$ using 100% SAF. This analysis shows a potential for Ryanair to decrease emissions by up to 81%. With Ryanair's aim to increase use of this SAF to a blending fraction of 40%, this becomes 60.02-63.34 gCO_2e/MJ_{SAF} or 46.39-48.98 $gCO2e/RPK$, which will contribute to their goal to reduce their emissions to under 60 $gCO2e/RPK$ by 2030, leading to a decrease in emissions by up to 32% compared to 100% Jet-A.

Key Words:

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1. Introduction

1.1. Motivation for Research

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.

Life cycle assessment (LCA) plays a very important role in decreasing aviation emissions. It 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. Synthesised fuels like biofuels produced from feedstocks such as rapeseed, canola, and camelina for example, absorb carbon from the atmosphere when grown, and it is later released back into the atmosphere when the finished fuel is burned. This means the combustion element of biofuels is net carbon zero [1]. However, when producing biofuels and renewable fuels, the emissions from feedstock cultivation, harvesting, and fuel production need to be considered.

LCA emissions are broken up into three sections. Well-to-Pump (WTP), Pump-to-Wake (PTW), and Well-to-Wake (WTW) emissions. Well-to-Pump emissions consider every step of the fuel production process, from initial cultivation of the feedstock to the refined fuel in the airport tank farm, Pump-to-Wake emissions represent solely the combustion emissions of the fuel, and Well-to-Wake emissions is the combined Pump-to-Wake and Pump-to-Wake emissions, the total emissions, and embodied emissions of the finished fuel. The unit used to measure these emissions is generally gCO_2e/MJ, where 'e' denotes equivalent. This contains non-CO_2 emissions, such as NO_x or CH_4. These gases are formed alongside CO_2 during combustion, feedstock cultivation, and other steps of the Well-to-Wake process. These gases have an assigned global warming potential, which standardise their warming potential in units of CO_2 [2].

In aviation, emissions can be reduced in several ways including SAF use, increasing operational efficiency, and technological advancements. Each of these factors contribute to cleaner aviation by reducing or replacing fossil fuel use. The scope of this study aims to incorporate each of these factors, by assessing a scenario analysis of Ryanair's operations.

SAF produced from waste or renewable sources is a promising low carbon fuel that is widely considered as a medium-term solution for combatting emissions and reducing fossil jet fuel dependency, while posing no disruption to existing jet fuel supply [3]. Currently, there are issues with SAF production despite its benefits in reducing emissions. They include; lack of availability, limited production facilities, technical uncertainties, policy uncertainties, public perception, economic considerations, and environmental impact of production and distribution [4-11]. Research in the LCA of SAF allows for a reduction in some of these uncertainties while quantifying the emissions savings associated with its use.

Specific scenario analysis is required for the LCA of SAF. Current life cycle assessment uses assumptions that represent general calculations. This is not enough to quantify an airlines potential emission reductions. Industry based calculations from information of the actual supply chain of the SAF, provided by companies such as Ryanair, Neste, and Exolem is needed to conduct a more accurate, scientific approach to life cycle assessment. It is also important to include the use of revenue passenger kilometre (RPK or Pax) in our LCA study, as it is beneficial towards LCA because it incorporates airline efficiency and total fuel use. Therefore, it is the aim of this project to incorporate real supply chain industry information for specific SAF use, and incorporate the use of RPK units into LCA, and to quantify the emissions of Ryanair's operations for specific scenario-based analysis.

1.2. Project Objectives

This project contains the following objectives:

1. To determine the greenhouse gas $CO_2(eq)/MJ_{SAF}$ emissions from Ryanair's sustainable aviation fuels using life cycle assessment.
2. Create TCD LCA greenhouse gas $CO_2(eq)/RPK$ model for Ryanair operations that can be used for different Ryanair Scenarios.
3. Use the TCD LCA model to determine Ryanair emission projections and determine whether they are aligned with their set goals.
4. Replicate and verify industry calculated LCA used by Ryanair with science-based assumptions and TCD methodology.

1.3. Science Based Targets

The Science Based Targets Initiative (SBTi) is a target setting methodology that provides a pathway for companies to reduce greenhouse gas emissions [12]. SBTi uses a company's emissions data to create short- and long-term emissions reductions goals. It is an incentive to promote the reduction of greenhouse gas emissions within industry. SBTi provide a roadmap for airlines to reduce emissions, with specific goals. However, the methodology to reduce emissions is up to the company. It is an aim of this project to assist in the methodological roadmap in Ryanair's emission reduction targets, SBTi or otherwise.

Initial analysis of SBTi shows the target setting methodology is very ambitious, with impossibly large emission reduction goals being set for hard to abate sectors such as aviation. Currently, Ryanair has set a near-term SBTi target [12], as well as personal targets that TCD will assist in mitigating.

1.4. Current Methodologies in LCA Assessment

1.4.1. CORSIA

There are different methodologies used by airlines in the LCA of SAF, CORSIA is one of them [2]. CORSIA is the Carbon Offsetting and Reduction Scheme for International Aviation and aims to form one unified LCA methodology in aviation internationally. The system boundary for CORSIA is shown in Figure 1, describing the different factors that are considered in their LCA.
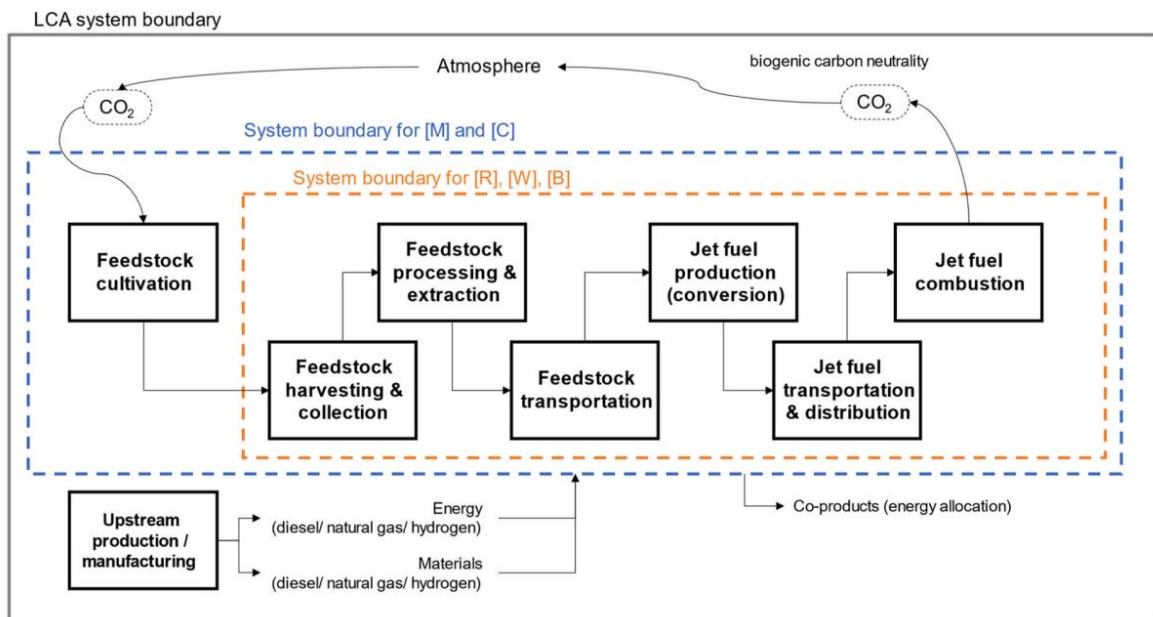

Figure 1: System boundary for CORSIA LCA methodology [2]. The feedstocks are categorized in different classifications, they are: main products [M], co-products [C], residues [R], wastes [W], and by-products [B].

Figure 2 shows the full list of CORSIA eligible fuels (CEF) with their default core LCA values compared to the petroleum jet fuel baseline. The default core LCA values for each CEF is a general calculation of the LCA of different SAFs. Different LCA tools and databases were used in these calculations.
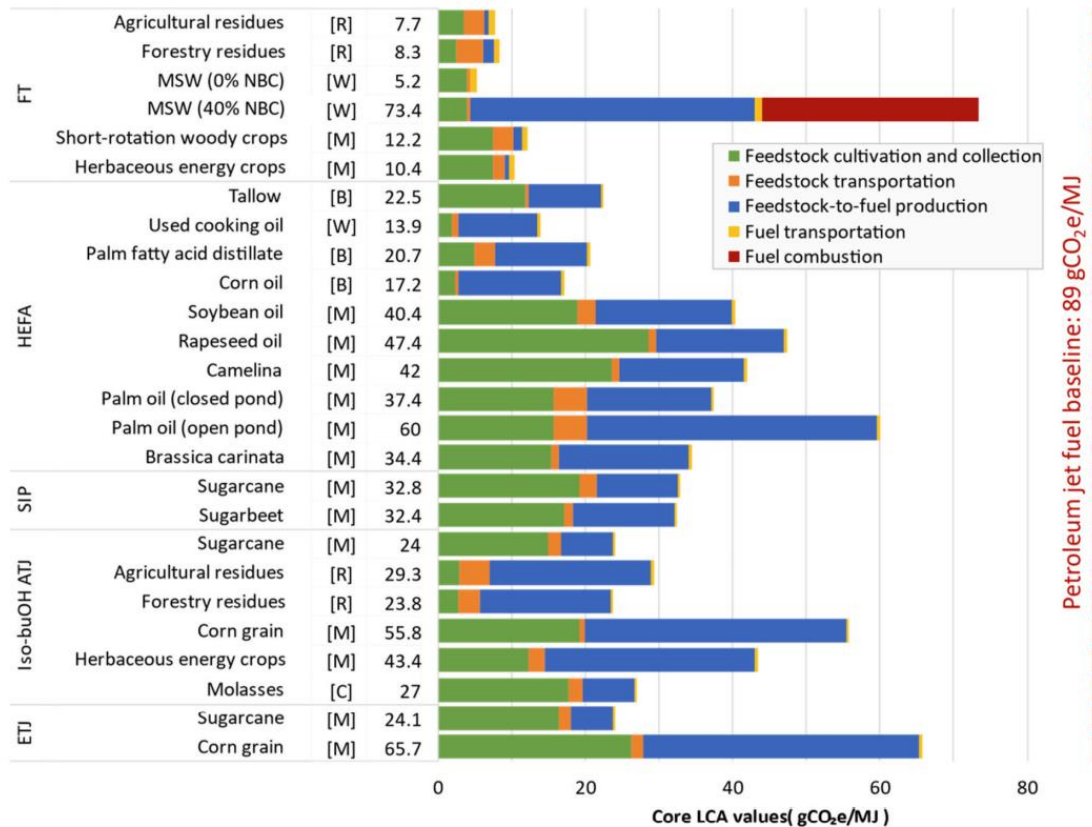
Figure 2: CORSIA default core LCA values of SAF production pathways approved by the International Civil Aviation Organization (ICAO) to date. Here NBC is non-biogenic content [2].

In CORSIA Supporting Document for LCA Methodology [13], the International Civil Aviation Organization (ICAO) describes the methods used in calculation of the default core LCA values. For example, for used cooking oil hydroprocessed renewable jet fuel; a modified Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model (GREET) [14] model created by Seber et al. [15] was used by Massachusetts Institute of Technology (MIT), in conjunction with the European Commission Joint Research Centre (JRC) using the E3 database life-cycle assessment tool. MIT calculated the LCA of hydroprocessed renewable jet fuel SAF from used cooking oil to be 14.8 gCO_2e/MJ, while JRC calculated 13 gCO_2e/MJ. These values were verified by Argonne National Lab (ANL). The average of these values was decided as the core default LCA value of hydroprocessed renewable jet SAF (13.9 gCO_2e/MJ) produced from used cooking oil. The data is summarised in Table 1:

Table 1: CORSIA LCA results for used cooking oil hydroprocessed renewable jet sustainable aviation fuel [gCO$_2$e/MJ$_{SAF}$] [16]. Two independent studies using different LCA tools calculated the emissions associated with each step in SAF production. The midpoint value combines the research in both studies to create the default core life cycle value for CORSIA.

Data Provider	Massachusetts Institute of Technology [17]	European Commission Joint Research Centre [18]
Model Used	GREET [15]	E3 Database (E3) [19]
Individual LCA steps	LCA value for each step (gCO$_2$e/MJ$_{SAF}$)	
Feedstock Cultivation and Collection	3.6	0
Feedstock Transportation	0.3	1.7
Feedstock-to-Fuel Conversion	10.5	11
Fuel Transportation	0.5	0.3
Total	14.8	13
Midpoint Value	13.9	

Table 1 provides a comparable example of current accepted individual LCA values for feedstock cultivation, fuel production, and transportation for SAF produced from waste materials. These figures are currently being used in CORSIA methodology [2].

From an initial read of the default core LCA values in Figure 2, it is clear there is a variance in LCA values depending on the feedstock and production method. The issue with the CORSIA methodology is these default core LCA values.

In the CORSIA methodology, an airline may claim emissions reductions from the use of CORSIA eligible fuels. Airlines may either accept the default core LCA values for emissions credits, or if they claim their emissions to be different than these values, they must submit an actual core life cycle value calculation. This report highlights that there is no one number for each section described in Table 1. More information on this calculation criteria is in the supplementary material.

The motivation behind the use of SAF is to reduce aviation emissions. Airlines need specific LCA calculations if they want to decarbonise. It is not enough to use the default core LCA values calculated by CORSIA, as they will not be specific to their operations. LCA calculation requires hundreds of specific inputs. Each of these inputs are variable depending on factors such as: feedstock supplier, fuel supplier, location of fuel rendering facilities, airport, airport operating procedures, aeroplane used, aeroplane route, blending mandates for airlines and airports. Each of these factors will be different for every flight in every airline. Each of these

factors influence the overall LCA value. Hence, specific LCA calculations for these factors need to be considered rather than relying on CORSIA's generalised default core LCA values.

1.4.2. EU ETS

The European Union Emissions Trading System (EU ETS) is an incentive for companies in Europe to reduce emissions. Like CORSIA, it involves a credit system where emissions trading can take place. The difference in EU ETS and CORSIA however is that the EU ETS scheme works as a monitoring system in a company's annual emissions. A company's total annual emissions are monitored and verified by the EU ETS. Depending on the company, the EU ETS gives an emissions allowance. If companies emit over their allowance they can face serious financial penalties [20]. The EU ETS is not an aviation specific ETS like CORSIA. It does not have default LCA values associated with SAF use. Therefore, it is very important that TCD provide the most accurate emissions calculation possible, by conduction an in depth LCA study of Ryanair operations and SAF use. As Ryanair travel mostly within the EU, this LCA result will assist in Ryanair's annual emissions reduction.

2. Literature Review

2.1. LCA Tools in Literature

A summary of the different LCA tools and a description of their possible LCA assessments are shown in Table 2. The Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model (GREET) [14], GHGenius [21], and BioGrace [22] are some of the most used LCA tools used in literature. They are open source, meaning their inputs can be changed and the tool modified. GREET and GHGenius are the most up to date LCA tools, as BioGrace has not been updated since 2015 to incorporate new RED II methodology [23]. These tools served as a basis for LCA calculation methodology in this project.

Other LCA tools not mentioned in Table 2 are Virtual Sugarcane Biorefinery (VSB) [24], SimaPro [25], the Environmental Policy Integrated Climate Model (EPIC) [26], and the Alternative Fuel Transportation Optimization Tool (AFTOT) [27]. VSB is an LCA tool developed by Brazilian Center for Research in Energy and Materials that specialises in sugarcane biorefinery configurations. In the case of Ryanair operations, it is not useful as the fuel being investigated is hydroprocessed renewable jet fuel. SimaPro is a LCA software used for the assessment of products, it is specialised for business use and is not open source. EPIC

is a tool that analyses agricultural soil to predict feedstock price, and AFTOT is a road transportation LCA tool. It is important to be aware of these tools and how they are used in literature to calculate hydrotreated renewable jet SAF greenhouse gas emissions, however, not all tools are applicable for this section of the LCA study, where the fuel production section is the primary focus. There are cases where these calculators have been used, or assist in hydroprocessed renewable jet fuel LCA calculations, however they are not specialised for this function in the same way GREET, GHGenius, and BioGrace are.

Table 2: Summary of LCA tools studied in this project: GREET [14], GHGenius [21], and BioGrace [22]. Here X denotes "Yes" that the tool can calculate the pathway in the columns in the left. A blank cell denotes "No". "*" denotes that the tool can be used in these cases, but the original tool was modified and the base tool is not capable of that pathway.

LCA Tool	GREET	GHGenius	BioGrace
Developer	Argonne National Lab	(S&T)[2]	Volunteer based
Funding	US government funding	internally funded	Co-funded by the Intelligent Energy Europe Programme of the European Union
Latest Release	2022	2021	2015
Default Region	USA	Canada	EU
Sustainable Aviation fuel Production Pathways			
Fischer-Tropsch	X		
Hydroprocessed Renewable Jet	X	X	X
Ethanol-to-Jet	X	X	
Sugar-to-Jet	X		
Hydroprocessed Renewable Jet feedstocks			
Soybean	X	X	
Palm	X	X	X
Canola	X	X	
Jatropha	X	X	
Camelina	X	X	
Algae	X	X	
Corn Oil	X	X	
Carinata	X		
Rapeseed			X
Sunflower			X
Used Cooking Oil	*	X	
Tallow	*	X	
Palm sludge oil		X	
SBE oil		X	
Fish oil		X	

Table 2 shows a breakdown of the different possible uses for GREET, GHGenius, and BioGrace. GREET specialises in more SAF production pathways, GHGenius has less

production pathways, but contains more feedstock sources, and BioGrace focuses on one production pathway with few feedstock sources.

A quick analysis of one pathway in the different LCA tools described above shows the variation of the default parameters in these calculators. Figure 3 displays the LCA of hydroprocessed renewable jet SAF from rapeseed oil and their comparison to CORSIA and the first Renewable Energy Directive (RED I).
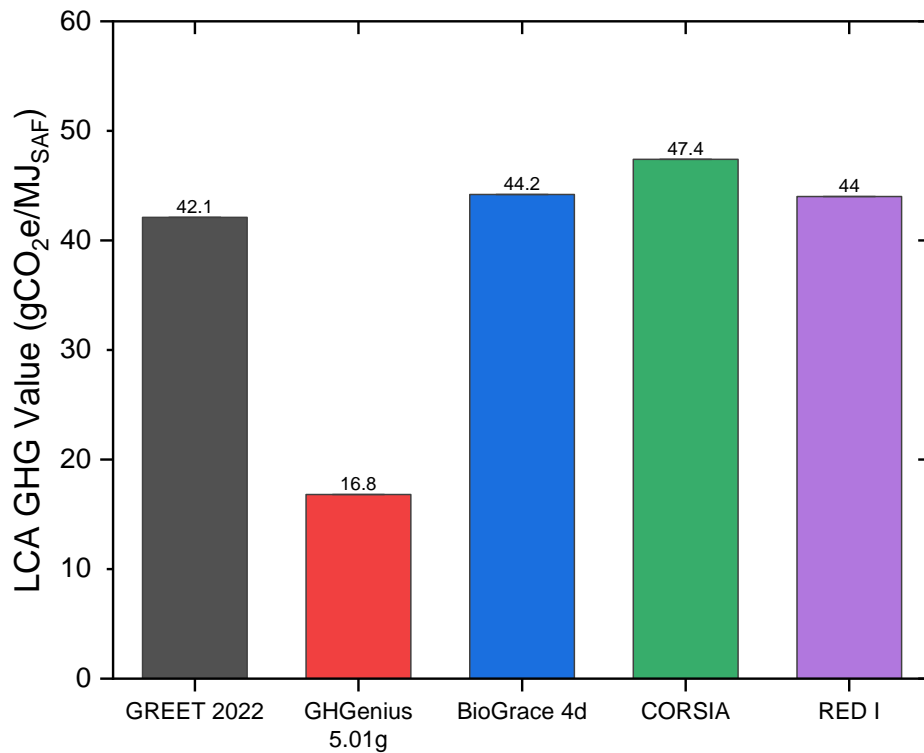

Figure 3: Comparison of the total default LCA value from different LCA calculators for rapeseed hydroprocessed renewable jet pathway compared to CORSIA [28] and RED I [29] in gCO$_2$e/MJ$_{SAF}$.

Here, GREET and BioGrace produce a calculated value similar to CORSIA and RED I, while GHGenius does not. This is due to a parameter in GHGenius that includes negative emissions due to co-product allocation. This feature is used in GREET, but the parameters around co-product allocation in GREET are fundamentally different, the effect it has on the final LCA value is not as influential as in GHGenius.

This shows extreme variation in different LCA calculators for almost identical pathways. Depending on the choice of model, the LCA value can be very different for the same feedstock, region, and co-product allocation methods. This highlights a need for specific inputs that are an actual representation of airline operations. When specific inputs are not sourced, a general

case LCA must be made. A general case LCA causes variation and uncertainty due to pre-programmed parameters that may not reflect the real-life scenario.

Current LCA tools do not represent specific scenarios without intense modification of the tool. Even with modification, the tools are very complex and difficult to decipher how exactly the LCA value is derived. This leads to inaccurate LCA values for specific scenarios where each detail matters. This could lead to airlines purchasing or investing in lesser quality and less sustainable SAF. It is important that LCA calculations are representative of airline operations and generalizing parameters is ultimately removed.

In GHGenius, it is possible to change the region-specific data to tailor results for specific areas. This feature is accurate for some countries, but in the case of the EU uses an average value. This does not take represent a company like Neste for example, who's refineries are in some of the greenest countries in Europe.

Neste, and other companies, invest heavily in feedstock to fuel conversion technology. The details of the material inputs for these processes are required for an accurate LCA calculation, however these processes are patented, and details are blocked by NDAs. Therefore, general values from literature based on Honeywell used cooking oil conversion technology is used in calculators, which further increases the uncertainties for specific emission savings.

There are other areas in LCA calculators than contain unnecessary uncertainty, for example, GREET uses a standard 737 single aisle aeroplane in its calculations. Ryanair has invested 22 billion USD in 210 new 737-8200 aircrafts, which are 16% more efficient than their current 233 737-800 aircrafts. GREET does not allow more than one plane to be considered in its analysis, which is what's needed to quantify Ryanair's operations.

The issue with the LCA calculators described above is that they do not accurately describe the scenario of a specific airline. It is considered that these LCA calculators are mostly open-source Excel models. This means that they can be modified, and numbers can be changed to better represent specific scenarios. However, eventually it becomes the case that calculating LCA values from first principles is not only more accurate, but simpler, as we control the calculation entirely, and no hidden parameters can effect the final calculation.

Furthermore, in the case of fuel production emissions alone, the inputs required in these calculators are: hydrogen use, natural gas use, electricity use, fossil fuel use, etc. These inputs are used directly to calculate greenhouse gas values from the emission factors of the fuels. This

is non-scientific, as the inputs are the most difficult numbers to source. It should not be reliant on the user. Depending on the feedstock used to produce SAF, different amounts of hydrogen, electricity, etc., are needed to transform that feedstock into SAF. What is needed in these models is a module that calculates these important inputs depending on feedstock selection, type of SAF to be produced, and where the fuel production facility is. From modelling the conversion of the feedstock to SAF on a molecular basis, these inputs can be estimated. This is something that is not in current LCA tools, and hence not in current LCA literature.

Other aspects that are not considered in LCA models is the use of revenue passenger kilometre (RPK) units. This is a unit that allows airlines to be rewarded on their efficiency, as load factor, total passengers, and total kilometres travelled is considered in the calculation.

This highlights the needs for a TCD calculator made from first principles. From studying these tools, analysing literature that use these tools for analysis of SAF, and reading literature that produce their own models, the most important aspects of LCA within these tools can be determined. The four areas we found to be most important in the building of our calculator is described in section 2.2.

2.2. LCA Literature Synopsis

The literature in LCA is dominated by studies focusing on variations of aspects such as feedstock, co-product allocation, land-use change, region, and the LCA tool used. These parameters are interchanged to describe different pathways in LCA studies using the same tool (See studies in Table 3). In other literature [30, 31], a combination of LCA tools are used to describe one or more pathways, similar to how CORSIA calculates their default core LCA values [13]. There are 14 LCA studies summarised in Table 3, eight used the LCA calculator GREET [14], two used GREET and the E3 database [19], one used SimaPro [25], one used Gabi [32], one used a combination the Environmental Policy Integrated Climate Model (EPIC) [26], and the Alternative Fuel Transportation Optimization Tool (AFTOT) [27], and two used their own model.

Table 3: Summary of hydroprocessed renewable jet total (HRJ) LCA values (gCO2e/MJ$_{SAF}$) depending on feedstock, allocation method, land use change (LUC) inclusion, refining method, product, and location [33].

Case	LCA Tool	LCA GHG emissions (gCO$_2$e/MJ)	Feedstock	Co-product allocation method	LUC inclusion	Refining technology	Product	Location	Source
1.	Own	67.3	Rapeseed	Displacement	No	Neste	Biodiesel	EUR	[34]
2.	GREET	54.9	Rapeseed	Energy	No	UOP	HRJ	ND/SD USA	[35]
3.	GREET	54	Rapeseed	Energy	No	UOP	HRJ	EUR	[36]
4.	GaBi	257.3	Rapeseed	Energy	Forestland	Neste	Biodiesel	EUR	[37]
5.	GREET and E3	47.4	Rapeseed	Energy	No	N/A	HRJ	N/A	[16]
6.	Own	60	Camelina	Displacement	No	UOP	HRJ	MT USA	[38]
7.	GREET	47	Camelina	Energy	No	UOP	HRJ	MT USA	[39]
8.	SimaPro	8.5	Camelina	Displacement	No	UOP	HRJ	SK CAN	[40]
9.	SimaPro	31	Camelina	Displacement	No	UOP	HRJ	SK CAN	[40]
10.	GREET and E3	42	Camelina	Energy	No	N/A	HRJ	N/A	[16]
11.	GREET	39.5	Soybean	Energy	No	UOP	HRJ	EUR	[36]
12.	GREET	37.5	Soybean	Energy	No	UOP	HRJ	USA	[41]
13.	GREET	34.12	Soybean	Displacement	No	UOP	Biodiesel	USA	[42]
14.	GREET	37	Soybean	Energy	No	UOP	HRJ	EUR	[35]
15.	GREET	97.8	Soybean	Energy	Grassland	UOP	HRJ	USA	[35]
16.	GREET	314.4	Soybean	Energy	Global Average	UOP	HRJ	USA	[41]
17.	GREET and E3	40.4	Soybean	Energy	No	N/A	HRJ	N/A	[16]
18.	GREET	44	Canola	Energy	No	UOP	HRJ	ND/SD USA	[43]
19.	SimaPro, EPIC, AFTOT	43	Canola	Displacement	No	UOP	HRJ	ND USA	[44]
20.	SimaPro, EPIC, AFTOT	-12	Canola	Displacement	Cropland	UOP	HRJ	ND USA	[44]
21.	SimaPro, EPIC, AFTOT	36	Canola	Energy	Cropland	UOP	HRJ	ND USA	[44]
22.	GREET	53	Canola	Energy	Forest	UOP	HRJ	MN CAN	[31]
23.	GHGenuis	41	Canola	Energy	Forest	UOP	HRJ	MN CAN	[31]
24.	GREET	48	Canola	Energy	No	UOP	HRJ	MN CAN	[31]
25.	GHGenius	38	Canola	Energy	No	UOP	HRJ	MN CAN	[31]
26.	GREET	27	Used Cooking Oil	Energy	N/A	UOP	HRJ	USA	[39]
27.	GREET	16.8	Used Cooking Oil	Energy	N/A	UOP	HRJ	USA	[15]
28.	GREET	19.4	Used Cooking Oil	Energy	N/A	UOP	HRJ	USA	[15]
29.	GREET	21.4	Used Cooking Oil	Energy	N/A	UOP	HRJ	USA	[15]
30.	GREET and E3	13.9	Used Cooking Oil	Energy	N/A	UOP	HRJ	USA	[16]

In cases 4, 15, 16, 20, 21, 22, and 23, land use change (LUC) was used. These studies show the range in how land use change emissions can completely alter LCA results. Take cases 12, 14, 15, and 16 for example. These studies all analysed the LCA of SAF from soybean oil, all using the GREET model. Two studies (cases 12 and 14) calculated the LCA of soybean oil to within 0.5 gCO$_2$e/MJ. This is expected as many parameters as possible in the study remain the same. Cases 15 and 16 calculate the same LCA value using land use change emissions and disagree by 60.3 and 276.9 gCO$_2$e/MJ compared to case 12. Cases 14 and 15 are two separate LCA's from the same study, with the difference being the inclusion of land use change in one case. The change in the LCA value is 60.8 gCO$_2$e/MJ, a 164% increase. The dramatic increase in the LCA value by the inclusion of one more parameter is the reason why land use change emissions are usually excluded in LCA in literature, in addition to not enough information about feedstock sourcing.

It is however possible to include land use change emissions and do it correctly. Cases 22-25 show a study where the LCA of canola from Manitoba Canada was calculated. This paper has the luxury of feedstock sourcing, with accurate information regarding land history, fertilizer use, soil properties, and exact location where the feedstock was grown. Cases 22-25 show the final LCA value for canola grown in the same region. Both GREET and GHGenius show little variation in the final LCA greenhouse gas value, however this is very minimal compared to other cases from the same study (14, 15). It remains the case that the information relating to feedstock sourcing is a luxury and is excluded in most LCA studies.

Waste materials are therefore the most beneficial feedstocks for reducing emissions in the feedstock production and procurement section of LCA, as land use change is not applicable. Waste materials include used cooking oil (UCO), tallow, agricultural residues, and others. The production emissions of these materials is not considered by current LCA methodologies [16] as the oils were originally produced for another purpose rather than SAF production, hence any land use change emissions bound to the waste products is the responsibility of the original producer, therefore only transportation emissions from collection and distribution of the feedstock are considered.

The most consistent low LCA emissions are hydroprocessed renewable jet fuel produced from used cooking oil, this is observed in cases 26-30. This highlights the role of waste materials in decarbonising aviation. Hydroprocessed renewable jet fuel technology is well developed for used cooking oil conversion to SAF. Neste and Honeywell are leading experts

in this area, however not much literature has data or information relating to Neste's NEXBTL conversion technology. This is another gap in literature that needs to be reported for accurate LCA reporting.

GREET is widely described in literature as the most prominent LCA calculator. Being open source, it allows the user to change inputs and observe calculations. Using GREET, other LCA tools, the studies in Table 3, other studies [15, 30, 33, 45-52], and TCD intuition, the TCD fishbone diagram analogy was created. It is designed to incorporate the most important aspects of LCA highlighted in literature and to include aspects of Ryanair's operations such as airport logistics and specific aircraft parameters. This fishbone diagram forms the skeleton of our first principles model.

The four sections deemed most important in the LCA of SAF include; feedstock production and procurement, fuel production, airport operations, and aircraft operations.
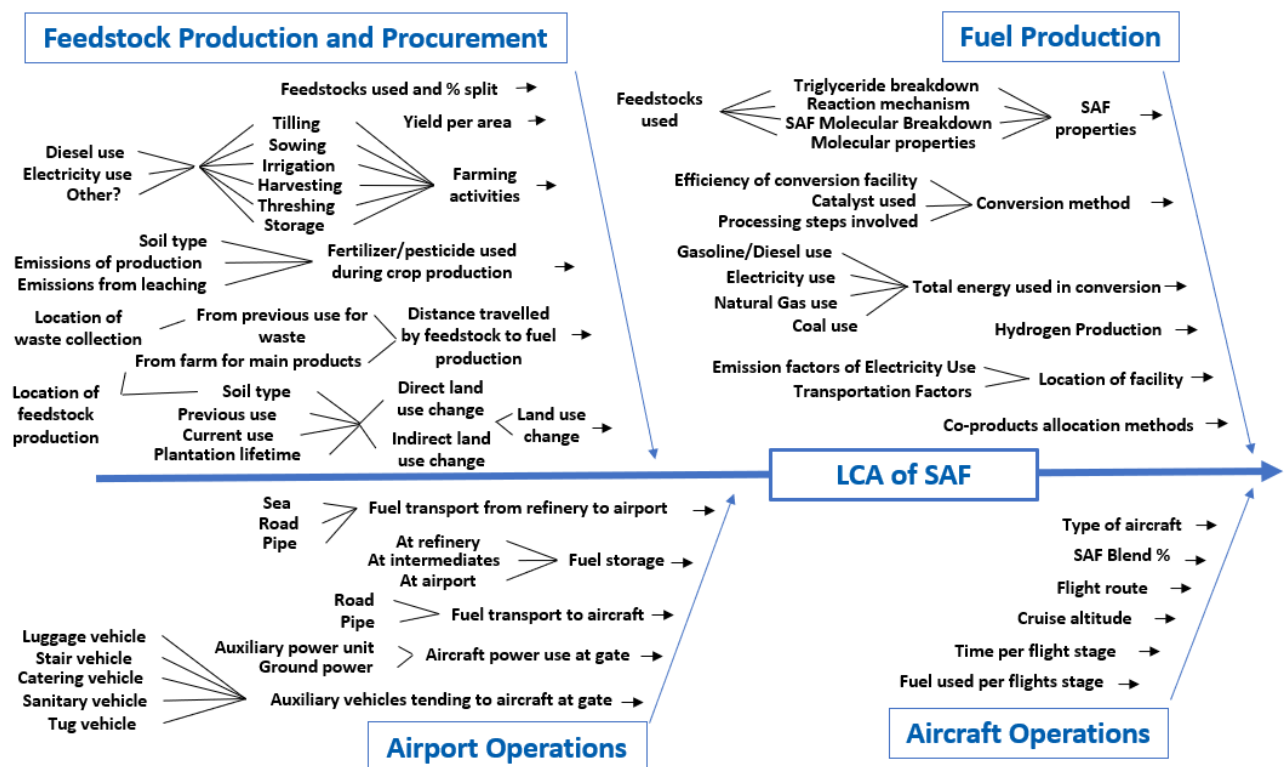

Figure 4: TCD Fishbone diagram of most important parameters in LCA work for quantitative assessment in literature. Each "bone" of the "fish" is a crucial area that need to be investigated, these are: Feedstock Production and Procurement, Fuel Production, Airport Operations, and Aircraft Operations.

The feedstock production and procurement fishbone contain areas related to feedstock cultivation, farming, fertilizer use, harvesting, land use change, and transport. For hydroprocessed jet fuel produced from waste materials however, this fishbone becomes smaller to contain transportation emissions of procurement and delivery to the fuel production facility only. Emissions associated with waste material production or prior use is not considered in this system boundary. This is in accordance with CORSIA LCA methodology [16].

The system boundary of the fuel production fishbone begins when the used cooking oil is delivered to the fuel production facility and ends when the competed SAF leaves the production facility for end use. Areas considered in this fishbone are feedstock used, conversion technology for that feedstock, total energy use in terms of gasoline/diesel, electricity, natural gas, and coal, emission factors associated with electricity use depending on location of production facility, and co-product allocation methods. The system boundary does not contain transportation emissions; however, transportation and distribution to and from the fuel production facility is considered in the other fishbones. This is to keep consistent methodology with all transportation emissions.

The airport fishbone contains emissions related to airport activity. It includes transportation emissions of SAF from the fuel production facility to the airport, non-fuel-embodied emissions from airport activities e.g. electricity use, and use of auxiliary vehicles. Transportation in this fishbone considers different modes of transport (pipeline, barge, road), and airport logistics in delivering fuel to the aircraft engine.

The aircraft fishbone incorporates aircraft parameters such as aircraft type, flight route, total fuel burned, and SAF blend used in the aircraft engine. An aspect also considered in this fishbone is the use of RPK units, hence passenger load factor is also considered.

Arvidsson et al. [34] and Agusdina et al. [38] used their own model to calculate LCA greenhouse gas emissions. Arvidsson et al. modelled Neste oil, for heavy duty vehicles. In their model, they considered production of vegetable oil in terms of farming emissions and field work operation, production of hydroprocessed renewable jet only in terms of electricity and hydrogen production, transport, and combustion of the fuel. Arvidsson did not consider energy use from fossil fuels in hydroprocessed renewable jet fuel production. Agusdina et al. used RPK units, and the Ecoinvent database for their LCA calculations altered with US regional data. This uses general data that does not specify aspects such as location of fuel production facility. This model did not consider aspects such as fossil fuel use [34], and locations of

individual facilities [38], which will be considered in the TCD LCA model, and this model was built for heavy duty vehicles, while the TCD LCA model considers the entire Ryanair supply chain, including heavy duty vehicles, but focuses on sustainable fuel use in planes.

It is the aim of this project to use real industry data in the analysis of Ryanair's operations. Real data was obtained from Ryanair, Neste, and Exolem and can be applied to the fishbone diagrams to reduce the number of assumptions made, thereby reducing uncertainty of the calculations and increasing the accuracy of the LCA of Ryanair's operations.

This report focuses on the fuel production element of the TCD LCA model. The feedstock, airport, and aircraft elements are governed by Aron Bell, my colleague on this project.

3. Methodology – Fuel Production Model

3.1. System Boundary - Ryanair Scenario 1

To make an accurate LCA of Ryanair's operations, we must define a scenario. The purpose of defining a scenario is to quantify the parameters to form a more specific and reliable LCA.

First, we define a simple case. The factors needed to be considered are the following: SAF use, Fuel burning intensity (defined by model of plane used, payload, and passenger load factor), airport logistics, and operational efficiency. From these factors, the aim is to calculate the total gCO_2e/RPK for this specific scenario. Here RPK is defined as "Revenue Passenger Kilometre", a unit used in aviation designed to include descriptive operational factors.

Ryanair Scenario 1 is defined as:
Route: Amsterdam Schiphol Airport (AMS) to Dublin Airport (DUB).
Aircraft: Boeing 737-8200.
Fuel: Neste Hydroprocessed Renewable Jet SAF (Made from 100% used cooking oil).

This scenario is agreed between TCD and Ryanair since April 2022. An aim of this project is to reduce greenhouse gas (GHG) emissions at airports. The route of Amsterdam to Dublin chosen by TCD gives the opportunity to calculate the greenhouse gas emissions of one complete flight, presenting results in gCO_2e/RPK rather than considering generic flight operations from Amsterdam. This route is also an active Ryanair route. The 737-8200 aircraft is chosen as it is the newest Ryanair aircraft. It seats more people, uses less fuel, and produced less noise than its predecessor.

The four areas to the Ryanair Scenario 1 LCA are feedstock, fuel production, airport, and aircraft. Figure 5 displays the Ryanair Scenario 1 fishbone with the parameters considered compared to the initial developed fishbone from Figure 4.

The green parameters are reliable data entry points from industry collaboration or accepted literature information, the orange parameters are parameters considered with well-established TCD assumptions, and the red parameters are factors not considered in our calculation. Red parameters are mainly found in the feedstock production and procurement fishbone as the feedstock is used cooking oil and only procurement emissions need to be accounted for.

Note here that the methodologies for the feedstock production and procurement, airport operations, and aircraft operations are not included in this report.
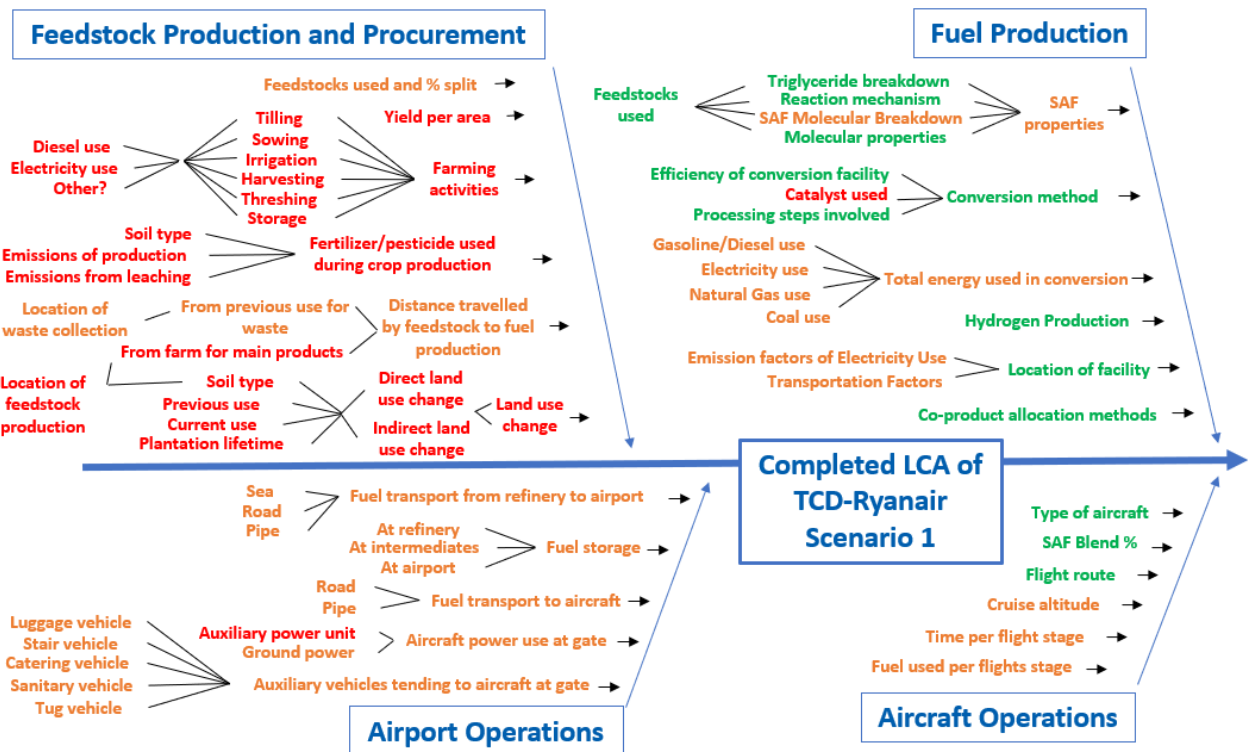

Figure 5: Initial Fishbone Diagram - Ryanair TCD LCA Scenario 1. This is Figure 4 altered to show what is considered in the TCD LCA model. The colour code is as follows: red denotes "Not considered", orange denotes "Considered – TCD Assumption", and green denotes "Considered – Verifiable".

3.2. Overview

Fuel Production is an integral part of the total Ryanair Scenario 1 LCA. It is the largest contributor to the final LCA result, and contains more variables, calculations, and complexity

than any of the other sections. Due to this, and the confidential nature of NESTE's fuel poduction process, it also requires more assumptions and thus more verification than any of the other individual model areas.

In this scenario, *Neste MY SAF* is the modelled fuel. Therefore, for fuel production it is assumed that the SAF is produced through the hydrogenation of vegetable oil (HVO) from waste products, and in this case 100% used cooking oil. The SAF is therefore hydrotreated renewable jet (HRJ). The system boundary for fuel production LCA is displayed in Figure 6.

The production process in Figure 6 was defined through examination of academic literature, namely from [33] and [51]. Here, the individual processing steps were researched, studied, and integrated into the calculation. It is the aim of this work to receive more specific information about processing from Neste to make the fuel production model as accurate as possible.
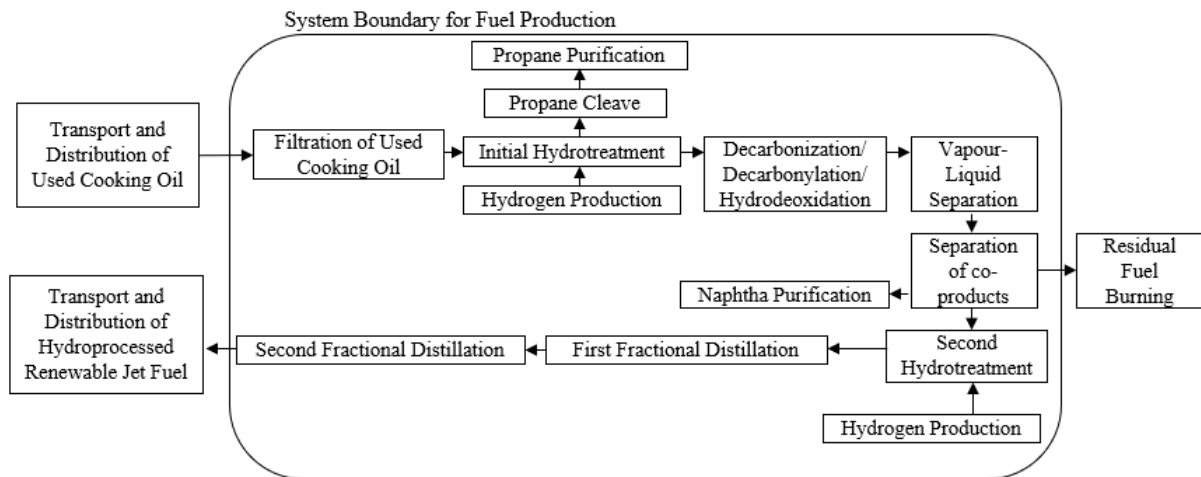

Figure 6: System boundary for fuel production in this study. A system boundary contains all the steps considered for analysis. The steps inside the system boundary produce and contribute emissions to the final LCA value for fuel production. The steps outside are either accounted for elsewhere in the final LCA, e.g., "Transport and Distribution", or is ignored due to assumptions, e.g., Residual Fuel Burning".

The steps in conversion considered in contribution to the total energy use are the following: filtration, initial hydrotreatment, propane cleave, deoxygenation/ decarbonisation/ hydrodeoxygenation, gas separation, second hydrotreatment (hydrocracking), fractional distillation, second fractional distillation, naphtha purification, and propane purification.
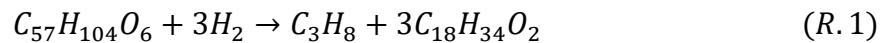
To determine the total emissions associated with fuel production, a mass and energy balance for each processing step was constructed. The aim of this mass and energy balance is to quantify the energy use in conversion of initial feedstock to hydroprocessed renewable jet. This is determined by following the flow of mass throughout the processing steps of Figure 6,

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observing the molecular changes, and calculating the energy use in each individual processing step.
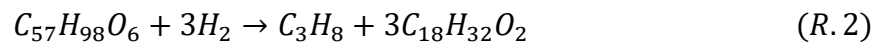
<mark>The initial feedstock is defined as used cooking oil. This can be represented in proportions of **triglycerides**, **diglycerides**, **monoglycerides**, and **free fatty acids**, as well as the individual **triglyceride** proportions of **triolein**, **trilinolein**, and **tripalmitin**.</mark> A reaction mechanism was defined according to these triglycerides in hydroconversion to free fatty acids, and their corresponding decarboxylation, decarbonylation, and hydrodeoxygenation reactions throughout the different processing steps previously defined in the system boundary. The reaction mechanism is shown in Equations R.1-R.14 below.
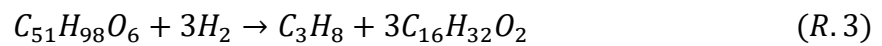
<u>Formation of fatty acids:</u>

Triolein + Hydrogen → Propane + Oleic acid

$$C_{57}H_{104}O_6 + 3H_2 \rightarrow C_3H_8 + 3C_{18}H_{34}O_2 \qquad (R.1)$$

Trilinolein + Hydrogen → Propane + Linoleic acid

$$C_{57}H_{98}O_6 + 3H_2 \rightarrow C_3H_8 + 3C_{18}H_{32}O_2 \qquad (R.2)$$

Tripalmitin + Hydrogen → Propane + Palmitic acid

$$C_{51}H_{98}O_6 + 3H_2 \rightarrow C_3H_8 + 3C_{16}H_{32}O_2 \qquad (R.3)$$

Oleic acid + Hydrogen → Stearic acid

$$C_{18}H_{34}O_2 + H_2 \rightarrow C_{18}H_{36}O_2 \qquad (R.4)$$

Linoleic acid + Hydrogen → Stearic acid

$$C_{18}H_{32}O_2 + 2H_2 \rightarrow C_{18}H_{36}O_2 \qquad (R.5)$$
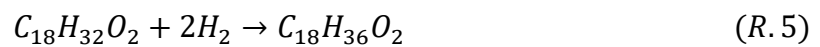
<u>Decarboxylation reactions:</u>

Stearic acid → Heptadecane + Carbon Dioxide
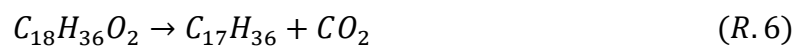
$$C_{18}H_{36}O_2 \rightarrow C_{17}H_{36} + CO_2 \qquad (R.6)$$

Oleic acid → Heptadecene + Carbon Dioxide

$$C_{18}H_{34}O_2 \rightarrow C_{17}H_{34} + CO_2 \qquad (R.7)$$

Palmitic acid → Pentadecane + Carbon Dioxide

$$C_{16}H_{32}O_2 \rightarrow C_{15}H_{32} + CO_2 \qquad (R.8)$$

Decarbonylation reactions:

Stearic acid + Hydrogen → Heptadecane + Carbon monoxide + Water
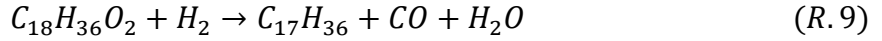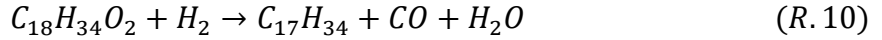
$$C_{18}H_{36}O_2 + H_2 \rightarrow C_{17}H_{36} + CO + H_2O \qquad (R.9)$$

Oleic acid + Hydrogen → Heptadecene + Carbon monoxide + Water

$$C_{18}H_{34}O_2 + H_2 \rightarrow C_{17}H_{34} + CO + H_2O \qquad (R.10)$$

Palmitic acid + Hydrogen → Pentadecane + Carbon monoxide + Water

$$C_{16}H_{32}O_2 + H_2 \rightarrow C_{15}H_{32} + CO + H_2O \qquad (R.11)$$

Hydrodeoxygenation reactions:

Stearic acid + Hydrogen → Octadecane + Water

$$C_{18}H_{36}O_2 + 3H_2 \rightarrow C_{18}H_{38} + 2H_2O \qquad (R.12)$$

Oleic acid + Hydrogen → Octadecane + Water

$$C_{18}H_{34}O_2 + 3H_2 \rightarrow C_{18}H_{36} + 2H_2O \qquad (R.13)$$

Palmitic acid + Hydrogen → Hexadecane + Water

$$C_{16}H_{32}O_2 + 3H_2 \rightarrow C_{16}H_{34} + 2H_2O \qquad (R.14)$$
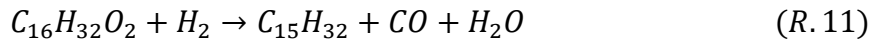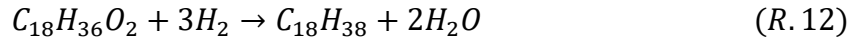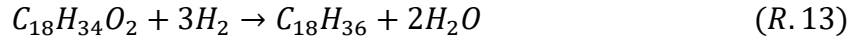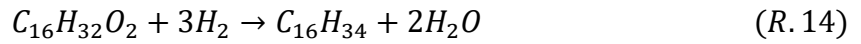
The reaction mechanism ends with a mixture of alkanes and alkenes ranging in carbon length C-15 to C-18. Next, the fuel mix is hydrocracked to a mixture of alkanes ranging from C-4 to C-18. The mixture is then fractionally distilled, and the products are separated according to their chain length. The products are: propane (C-3), LPG (C-4 to C-5), naphtha (C-6 to C-8), hydroprocessed renewable jet (C-8 to C-15), biodiesel (C-17 to C-18), residual oil (C-18+), hydrogen, water, carbon monoxide, and carbon dioxide.

The total energy in fuel production is the sum of the energy use for each processing step defined in the system boundary. The calculation of the energy use in each of these steps is described in section 3.2. The assumptions for each processing step is listed in the appendix. 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 were taken

from literature sources [53, 54]. For the electricity use, four different countries/regions were considered: Finland, Sweden, EU, and the Netherlands. <mark>Currently, the model is set to use 100% electricity, as it is an assumption that contributes the least uncertainty</mark>. The fuel production facility was chosen to be Finland as Neste has production and upgrading facilities in operation there.

3.3. Mass and Energy Balance

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 [33, 51, 55-59]. 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 equations and the assumptions in the appendix lead to the results published in section 4.2.

The net energy E_{Net} (J) is described in Equation 3.1. This is the total energy required for total conversion of used cooking oil to SAF and co-products.

$$E_{\text{Net}} = E_{\text{Total}}/\eta_{\text{System}} \qquad (Equation\ 3.1)$$

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 3.7-3.13. 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 3.7-3.13 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, $E_{T\text{otal}}$ (J), is the sum of each energy used in each of the processing steps in the feedstock to fuel conversion.

$$E_{Total} = E_{\text{Filtration}} + E_{\text{Initial Hydrotreatment}} + E_{\text{Propane Cleave}} + E_{\text{Deoxygenation/Decarbonisation}}$$
$$+ E_{\text{Vapour-Liquid Separation}} + E_{\text{Second Hydrotreatment}} + E_{\text{Fractional Distillation 1}}$$
$$+ E_{\text{Fractional Distillation 2}} + E_{\text{Naphtha Purification}} + E_{\text{Propane Purification}}$$
$$+ E_{\text{Residual Fuel Burning}}$$

$$(Equation\ 3.2)$$

The energy required for filtration, $E_{\text{Filtration}}$, (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:

$$E_{\text{Filtration}} = E_{\text{Triolein}} + E_{\text{Trilinolein}} + E_{\text{Tripalmitin}} + E_{\text{Unknowns}} \qquad (Equation\ 3.3)$$

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

$$E_{\text{Triolein}} = m_{\text{Triolein}} C_{p_{\text{Triolein}}} \left(T_f - T_i \right) \qquad (Equation\ 3.4)$$

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 3.4 is used to calculate the energies for each molecule in Equation 3.3. E_{Unknowns} (J) uses an average specific heat capacity of the molecules present in used cooking oil in Equation 3.4. The mass proportions found in Sotelo-Boyás et al [51] describe the mass% of each triolein, trilinolein, tripalmitin, and unknowns in used cooking oil.

The heat capacities of the are from Morad [55]. 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 [55].

The initial hydrotreatment energy, $E_{\text{Initial Hydrotreatment}}$ (J), follows the same methodology as $E_{\text{Filtration}}$ (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 [51, 52].

Equation 3.5 describes the energy used in removing propane from the reaction chamber, $E_{\text{Propane Cleave}}$ (J).

$$E_{\text{Propane Cleave}} = r_{VL}\left(m_{\text{C}_3\text{H}_8} + m_{\text{C}_3\text{H}_8\text{ Unknown}}\right) \qquad (Equation\ 3.5)$$

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 [59], $m_{\text{C}_3\text{H}_8}$ (kg) is the known mass of propane in the reaction chamber, derived from the reaction mechanism, and $m_{\text{C}_3\text{H}_8\text{ Unknown}}$ (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 3.1 as they are similar molecules. Therefore, it is assumed that a certain percentage of the unknows 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).

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

$$(Equation\ 3.6)$$

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 3.7) 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 3.7, describes the heat lost (Q (J/s)) between a liquid fuel and its environment.

$$Q = hA\left(T_{fuel} - T_{env}\right) \qquad (Equation\ 3.7)$$

Where,

$$h = \frac{q}{\Delta T} \qquad (Equation\ 3.8)$$

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 [60].

$$\frac{1}{h} = \frac{1}{h_{Trilinolein}} + \frac{1}{h_{Heptadecane}} \qquad (Equation\ 3.9)$$

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

$$h \cong q \qquad (Equation\ 3.10)$$

And therefore,

$$\frac{1}{q} = \frac{1}{q_{Trilinolein}} + \frac{1}{q_{Heptadecane}} \qquad (Equation\ 3.11)$$

And,

$$Q = qA(T_{fuel} - T_{env}) \qquad (Equation\ 3.12)$$

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

$$E_{Heating,\ Processing\ Step} = Qt = qA(T_{fuel} - T_{env})t \qquad (Equation\ 3.13)$$

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:

$$E_{Propane\ Cleave} = r_{VL}(m_{C_3H_8} + m_{C_3H_8\ Unknown}) + E_{Heating,\ Propane\ Cleave} \qquad (Equation\ 3.14)$$

In the current methodology, the heating calculations in Equations 3.7-3.13 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 3.1, and for processing steps that only require heating; Deoxygenation/Decarbonisation, 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 3.1. With more information from industry, the model can be improved by using Equations 3.7-3.13 in future.

The energy for vapor-liquid separation, $E_{\text{Vapor-Liquid Separation}}$ (J), is shown in Equation 3.15. CO_2, CO, H_2, H_2O, and C_3H_8 are produced through the reaction mechanism described in section 3.1. The CO_2, 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.

$$E_{\text{Vapor-Liquid Separation}} = r_{CO_2}\left(m_{CO_2}\right) + r_{VL}\left(m_{CO} + m_{H_2O} + m_{C_3H_8} + m_{H_2}\right) \quad (Equation\ 3.15)$$

Where r_{CO_2} (kJ/kg) is the rate of energy use for vapor-liquid separation for CO_2, r_{VL} (kJ/kg) is the rate of energy use for vapor-liquid separation defined in Equation 3.5, and $m_{Molecule}$ (kg) is the mass of the various molecules. CO_2 has a separate rate of energy use as in Zhang et al [59] compared to the other gases as CO_2 uses more energy per kg due to the energy required in carbon capture and storage. It is assumed that the intrinsic CO_2 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 3.16 describes the total mass and composition of Naphtha, m_{Naptha} (kg). The naphtha must then be purified. The energy use in naphtha purification is defined according to Equation 3.17.

$$m_{\text{Naptha}} = m_{C_8H_{18}} + m_{C_7H_{16}} + m_{C_6H_{14}} \qquad (Equation\ 3.16)$$

$$E_{\text{Naphtha Purification}} = p_N \times m_{\text{Naptha}} \qquad\qquad (Equation\ 3.17)$$

here, p_N (kJ/kg) is the energy required for purification [57]. 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 3.19).

Similarly, the mass of the propane formed in the reaction mechanism is described in Equation 3.18, and the energy use in propane purification is defined in Equation 3.19.

$$m_{\text{Propane}} = m_{C_3H_8} + m_{C_3H_8\ \text{Unknown}} \qquad\qquad (Equation\ 3.18)$$

$$E_{\text{Propane Purification}} = p_N \times m_{\text{Propane}} \qquad\qquad (Equation\ 3.19)$$

The residual fuel burning energy, $E_{\text{Residual Fuel Burning}}$ (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 gCO_2e/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 gCO_2e/MJ_{SAF} is the standard value used in SAF LCA and is defined as the total gCO_2e 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 [61]. 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, as we assume the fuel production facility is in Neste's Finland site.

The calculation process to standardize the net energy per 100kg used cooking oil (UCO) to gCO_2e/MJ_{SAF} is:

$$E_{Net} \frac{[\text{MJ}]}{[100 \text{ kg UCO}]} \rightarrow \frac{E_{Net}}{Yield_{SAF}} \frac{[\text{MJ}]}{[\cancel{100 \text{ kg UCO}}]} \frac{[\cancel{100 \text{ kg UCO}}]}{[\text{kg SAF}]}$$

$$\rightarrow \frac{E_{Net}}{Yield_{SAF} \times LHV_{SAF}} \frac{[\cancel{\text{MJ}}][\cancel{\text{kg SAF}}]}{[\cancel{\text{kg SAF}}][\cancel{\text{MJ}}]}$$

$$\rightarrow \left(\frac{E_{Net}}{Yield_{SAF} \times LHV_{SAF}} \right) \times EF_{grid}[\text{gCO}_2\text{e/MJ}]$$

$$= \text{Total gCO}_2\text{e/MJ}_{SAF} \text{ from energy use} \qquad (Formula \ 3.20)$$

The intrinsic CO_2 is formed as part of the reaction mechanism in section 3.1. Similarly to how the energy is standardized in Formula 3.19, the intrinsic CO_2 must be converted to $\text{gCO}_2\text{e/MJ}_{SAF}$.

$$CO_{2\,Intrinsic} \frac{[\text{g CO}_2]}{[100 \text{ kg UCO}]} \rightarrow \frac{CO_{2\,Intrinsic}}{Yield_{SAF}} \frac{[\text{g CO}_2]}{[\cancel{100 \text{ kg UCO}}]} \frac{[\cancel{100 \text{ kg UCO}}]}{[\text{kg SAF}]}$$

$$\rightarrow \frac{CO_{2\,Intrinsic}}{Yield_{SAF} \times LHV_{SAF}} \frac{[\text{g CO}_2][\cancel{\text{kg SAF}}]}{[\cancel{\text{kg SAF}}][\text{MJ}]}$$

$$= \text{Total gCO}_2\text{e/MJ}_{SAF} \text{ from intrinsic CO}_2 \qquad (Formula \ 3.21)$$

Hydrogen is consumed as part of the reaction mechanism in section 3.1. The production of this hydrogen is considered in the LCA of the SAF production. Like the Formula 3.20 and 3.21, the total hydrogen use must be standardized:

$$H_2 \frac{[\text{kg}]}{[100 \text{ kg UCO}]} \rightarrow \frac{H_2}{Yield_{SAF}} \frac{[\text{kg } H_2]}{[\cancel{100 \text{ kg UCO}}]} \frac{[\cancel{100 \text{ kg UCO}}]}{[\text{kg SAF}]}$$

$$\rightarrow \frac{H_2}{Yield_{SAF} \times LHV_{SAF}} \frac{[\text{kg } H_2][\cancel{\text{kg SAF}}]}{[\cancel{\text{kg SAF}}][\text{MJ}]}$$

$$\rightarrow \left(\frac{H_2}{Yield_{SAF} \times LHV_{SAF}} \right) \times EF_{Hydrogen\ Production} \frac{[\text{kg } H_2]}{[\text{MJ}]} \left[\frac{\text{g CO}_2\text{e}}{\text{kg } H_2} \right]$$

$$= \text{Total gCO}_2\text{e/MJ}_{SAF} \text{ from hydrogen use} \qquad (Formula \ 3.22)$$

The total gCO2e/MJ$_{SAF}$ for fuel production is calculated by the following equation.

$$\text{Total CO}_2\text{e/MJ} =$$

$$\text{Total gCO}_2\text{e/MJ}_{SAF} \text{ from energy use} + \text{Total gCO}_2\text{e/MJ}_{SAF} \text{ from intrinsic } CO_2$$

$$+\text{Total gCO}_2\text{e/MJ from hydrogen use} \qquad (Equation \ 3.23)$$

Equations 3.24 and 3.25 show the energy and mass allocation methodology used in Figure 10.

$$GHG_{\text{Energy Allocation}} = \text{Total gCO}_2\text{e/MJ [gCO}_2\text{e/MJ]} \times \left(\frac{m_{SAF} \times LHV_{SAF}[MJ]}{\text{Total E }[MJ]}\right)$$

$$(Equation\ 3.24)$$

$$GHG_{Mass\ Allocation} = \text{Total gCO}_2\text{e/MJ [gCO}_2\text{e/MJ]} \times \left(\frac{m_{HRJ}[kg]}{\text{Total } m\ [kg]}\right)$$

$$(Equation\ 3.25)$$

where,

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

$$(Equation\ 3.26)$$

and,

$$\text{Total m }[kg] = m_{Naphtha} + m_{SAF} + m_{Diesel} + m_{Residual\ Oil} + m_{Propane} + m_{LPG}$$

$$(Equation\ 3.27)$$

3.4. Conversion of gCO₂e/MJ to gCO₂e/RPK

The total emissions for this scenario are calculated by addition of the emissions from each section in Figure 4. The result is presented as gCO_2e/MJ of SAF. In commercial aviation, the unit of total CO_2e emissions per revenue passenger kilometre (gCO_2e/RPK) is used to standardise the emissions produced by how many passengers are on board, and how far the plane is travelling. This measure allows for a better description of how sustainable a specific flight is, as it considers passenger load and total fuel burned during the flight. By using this measurement, each passenger obtains a carbon footprint associated with that flight. This number is used by the airline to determine their greenhouse gas (GHG) efficiency, and by the passenger to have a record of their emissions, which are important for passengers travelling for business. The direct emissions of SAF combustion in the aircraft are neglected. This is due to the assumption that all greenhouse gas emissions are biogenic as they were previously sequestered during feedstock growth, before being processed into cooking oil.

First, the theoretical operational emissions of this scenario, using a 100% SAF blend, is calculated by determining the quantity of CO_2e emissions from operation of the flight. The fuel energy, E_{fuel} (MJ), used during the flight is calculated by multiplying the total mass of fuel used during the flight, m_{fuel} (kg), by the lower heating value/energy density of the SAF, LHV_{SAF} (MJ/kg), shown in Equation 3.28. The previously calculated gCO_2e/MJ_{SAF} is then multiplied by E_{fuel} (MJ) to find the total greenhouse gas emissions of the flight (gCO_2e) (Equation 3.29). The total emissions are divided by the number of passengers onboard the aircraft and the distance travelled, as shown in Equation 3.30. The number of passengers is calculated by assuming a 96% load factor in the 197-seat aircraft, as per the 2019 Ryanair average load factor [62]. This returns the flight's emissions in the form gCO_2e per revenue passenger kilometre (gCO_2e/RPK) (Equation 3.30).

$$E_{fuel}[MJ] = m_{fuel}[kg] \times LHV_{SAF}\left[\frac{MJ}{kg}\right] \qquad (Equation\ 3.28)$$

$$\text{Total flight emissions } [gCO_2e] = \text{LCA GHG Value}\left[\frac{gCO_2e}{MJ}\right] \times E_{fuel}\ [MJ] \quad (Equation\ 3.29)$$

$$\text{Total GHG emissions }\left[\frac{gCO_2e}{RPK}\right] = \frac{\text{Total flight } [gCO_2e]}{\#\text{Passengers} \times \text{distance travelled [km]}} \ (Equation\ 3.30)$$

It is assumed that the SAF is used at a 40% blend with Jet-A. This is the blend % that Ryanair plan to use for this scenario [62]. The equivalent gCO_2e/MJ and gCO_2e/RPK of this blend is calculated by the following Equations 3.31 and 3.32. The CORSIA accepted LCA value of 89 gCO_2e/MJ is used for Jet-A [28], and the gCO_2e/RPK of Jet-A is calculated by the same methodology as Equations 3.28-3.30.

$$\frac{gCO_2e}{MJ}\text{ of 40\% SAF Blend} = \left(\frac{gCO_2e}{MJ}\text{SAF} \times 40\%\right) + \left(\frac{gCO_2e}{MJ}\text{Jet-A} \times 60\%\right)(Equation\ 3.31)$$

$$\frac{gCO_2e}{RPK}\text{ of 40\% SAF Blend} = \left(\frac{gCO_2e}{RPK}\text{SAF} \times 40\%\right) + \left(\frac{gCO_2e}{RPK}\text{Jet-A} \times 60\%\right)(Equation\ 3.32)$$

4. Results

The results of the mass and energy balance are shown in Table 4. The products of the hydrocracked alkanes are divided into propane (C-3), LPG (C-4 to C-5), naphtha (C-6 to C-8),

jet fuel (hydroprocessed renewable jet) (C-8 to C-15), diesel (C-17 to C-18), residual oil (C-18+), hydrogen, water, carbon monoxide, and carbon dioxide.

Table 4: 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.

Mass and Energy Balance Results		
Description	Value	Unit
Naphtha	14.08	kg
Jet Fuel	56.47	kg
Diesel	5.37	kg
Residual Oil	0.00	kg
Water	6.53	kg
Propane	4.18	kg
LPG	8.62	kg
Carbon Dioxide	5.07	kg
Carbon Monoxide	3.23	kg
Spare Hydrogen	6.44	kg
Total	110.00	kg
Jet Fuel Yield	56.47%	% (kg SAF/ kg used cooking oil)

Table 5: Total LCA emissions for each processing step in the system boundary, with total emissions for fuel production with no co-product allocation methods, mass-based co-product allocation, and energy-based co-product allocation. Note here some values in the production step contribute 0.00 gCO2e/MJ$_{SAF}$, this is due to heat loss assumptions. See Section 3.1 under Equation 3.14 for more details.

Results		
Description of CO2e Source	Value	Unit
Filtration	0.41	gCO$_2$e/MJ(SAFe)
Initial Hydrocracking	2.05	gCO$_2$e/MJ(SAFe)
Propane Cleave	0.16	gCO$_2$e/MJ(SAFe)
Deoxygenation / Decarbonisation / Hydrodeoxygenation	0.00	gCO$_2$e/MJ(SAFe)
Vapour-Liquid Separation	1.21	gCO$_2$e/MJ(SAFe)
Propane Purification	0.16	gCO$_2$e/MJ(SAFe)
Water Removal/ Separation of Co-Product Gases	0.33	gCO$_2$e/MJ(SAFe)
Second Hydrotreatment	0.00	gCO$_2$e/MJ(SAFe)
Fractional Distillation 1	0.00	gCO$_2$e/MJ(SAFe)
Fractional Distillation 2	0.00	gCO$_2$e/MJ(SAFe)
Naphtha Purification	0.55	gCO$_2$e/MJ(SAFe)
Intrinsic CO$_2$	2.05	gCO$_2$e/MJ(SAFe)
Hydrogen Production	17.12	gCO$_2$e/MJ(SAFe)
Total Emissions from Fuel Production	24.05	gCO$_2$e/MJ(SAFe)
Total Emissions Using Mass Based Allocation	15.14	gCO$_2$e/MJ(SAFe)
Total Emissions Using Energy Based Allocation	15.31	gCO$_2$e/MJ(SAFe)

Table 5 shows a summary of the emissions from each individual processing step. The result of the total fuel production energy is 24.05 gCO_2e emitted per MJ of SAF. This is the total greenhouse gas LCA emissions of the fuel production process with no allocation method. Using energy allocation (Equation 3.24), this becomes 15.31 gCO_2e/MJ_{SAF}, and with mass allocation (Equation 3.25) this becomes 15.14 gCO_2e/MJ_{SAF}.

The results of Ryanair Scenario 1 are displayed in Table 6 below. The feedstock result is dependent on the used cooking oil origin. The four countries modelled are where Neste sources their used cooking oil: Indonesia, USA, China, and Germany. The default case of Indonesian used cooking oil using energy allocation is chosen as Neste source most of their used cooking oil from Indonesia, and energy allocation is the most practiced and accepted method for co-product allocation in literature (see Table 3).

Table 7 displays the results of Ryanair Scenario 1 in gCO_2e/RPK. The default feedstock source region is Indonesia, and the default production emissions allocation method is energy allocation.

Table 6: Total embodied emissions from Ryanair Scenario 1. This table combines the four areas described in the TCD LCA fishbone diagram. The feedstock, fuel production, and emissions are summed to give a total gCO_2e/MJ_{SAF} for each feedstock source, with one or more allocation methods.

Total Embodied SAF GHG Emissions	TCD Indonesia		TCD USA	TCD China	TCD Germany	Units
	No Allocation	Energy Allocation				
Feedstock	7.33	7.33	3.24	8.95	0.65	gCO_2e/MJ_{SAF}
Fuel Production	24.05	15.31	15.31	15.31	15.31	gCO_2e/MJ_{SAF}
Airport	0.60	0.60	0.60	0.60	0.60	gCO_2e/MJ_{SAF}
Total	31.97	23.23	19.15	24.85	16.56	gCO_2e/MJ_{SAF}

Table 7: Total embodied emissions per RPK for varying SAF blends. The results for "TCD Indonesia Energy Allocation" described in Table 6 is converted from gCO_2e/MJ_{SAF} to gCO_2e/RPK using information from the aircraft section of the fishbone diagram in Figure 5.

Total Emissions per RPK for Varying SAF Blends	TCD Indonesia Energy Allocation	Units
100% Jet-A	68.69	gCO2e/RPK
40% SAF, 60% Jet-A	48.48	gCO2e/RPK
100% SAF	18.18	gCO2e/RPK

5. Discussion

The result of the fuel production model shows the default parameter value 15.31 gCO_2e/MJ_{SAF} (Indonesia used cooking oil with energy allocation), is embodied in the production of the SAF used in Ryanair Scenario 1.

Figure 7 shows the comparison of the total greenhouse gas emissions from feedstock to hydroprocessed renewable jet calculated in the fuel production model compared to Neste, LCA calculators, literature, and policy values. Here "TCD" represents the fuel production results from Table 6. The red bars are fuel production emissions applied with energy-based allocation (See Equation 3.23), the blue bar is fuel production emissions with mass-based allocation (See Equation 3.24), the black bar is total fuel production emissions with no allocation, and the green bars are total LCA values. The label below (TCD, Neste, etc.) displays the author of that LCA value.
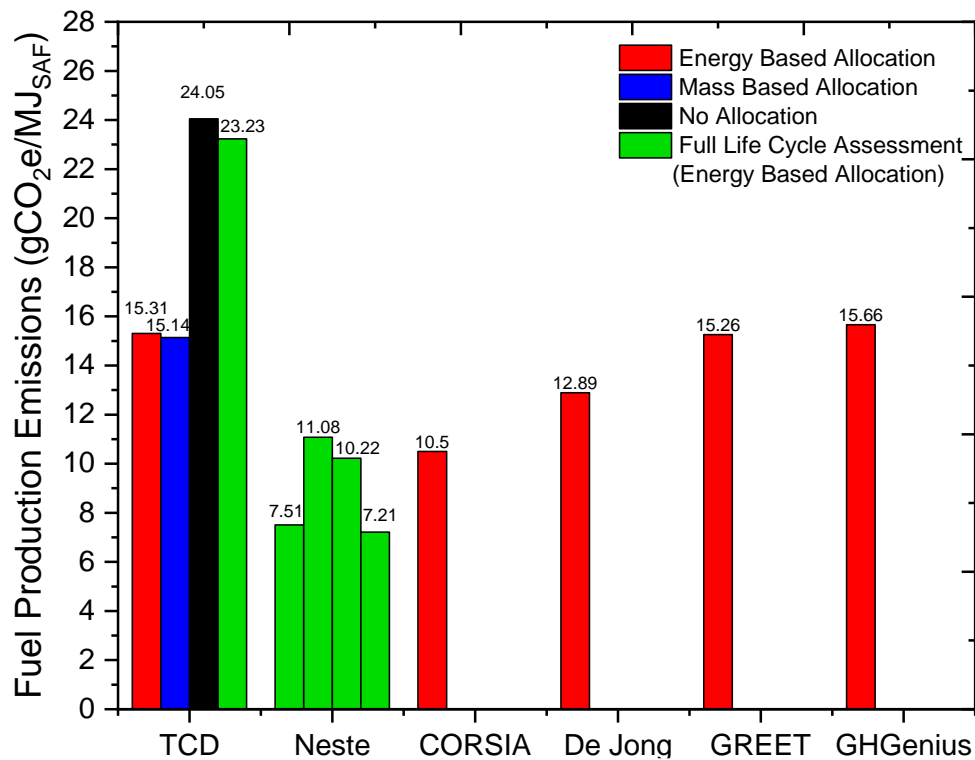
Figure 7: Comparison of production emissions from TCD derived value compared to LCA calculator GHGenius [21], Seber et al.'s modified GREET [15], literature value from De Jong et al. [39] and CORSIA [2]. Neste's certified LCA of 7.21, 7.51, 10.22, and 11.08 gCO_2e/MJ_{SAF} [63, 64] for used cooking oil hydroprocessed renewable jet SAF sourced from Germany, Indonesia, China, and USA respectively. Red coloured bars represent just fuel production emissions of TCD, CORSIA, De Jong, GREET, and GHGenius's LCA with energy-based allocation. Blue coloured bar represents just fuel production emissions of TCD's LCA with mass-based allocation. Black coloured bar represents just fuel production emissions of TCD's LCA with no allocation method. Green coloured bars are the total value of TCD's Indonesia energy-allocation LCA, and each of Neste's energy allocation LCA from Germany, Indonesia, China, and USA respectively from left to right.

The derived TCD LCA (23.23 gCO$_2$e/MJ$_{SAF}$ for used cooking oil SAF from Indonesia) is around three times Neste's final LCA for the same product (7.51 gCO$_2$e/MJ$_{SAF}$). Note here Neste's LCA values have undergone verification and certification. This is very surprising, as the fuel production section in CORSIA, De Jong, GREET, and GHGenius, and TCD's LCA are higher than Neste's entire LCA calculation.

This highlights the lack in information from industry, as assumptions needed to be made to estimate how Neste's NEXBTL conversion technology [64] works. This is the gap in literature clearly defined. There is no study that accurately describes a Neste certified LCA in literature. This is the motivation to partner with industry and together further develop accurate LCA, as well as utilising the LCA with actual fuel burning/aviation data directly from Ryanair to provide an accurate gCO$_2$e/RPK values that they can use to decarbonise. When this methodology is submitted to Gold Standard [65] and fully verified, it will become a one of kind study that is representative of industry engagement in LCA.

Total Embodied SAF GHG Emissions for Ryanair Scenario 1 (gCO$_2$e/MJ$_{SAF}$)
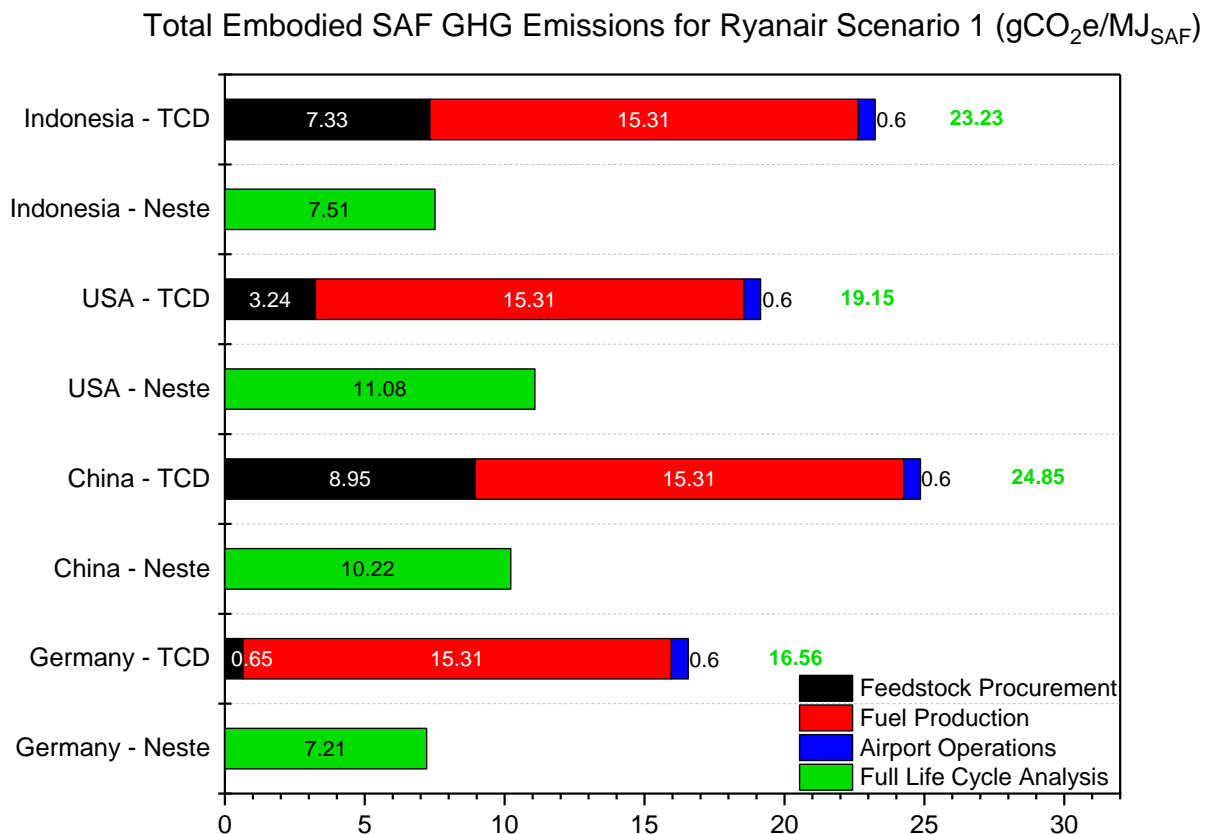
Figure 8: Total Embodied SAF greenhouse gas Emissions for Ryanair Scenario 1 using compared to Neste's claimed values [63, 64]. Black bars represent TCD's calculated LCA emissions from feedstock production and procurement. Red bars represent TCD's calculated LCA emissions from fuel production. Blue bars represent TCD's calculated LCA emissions from airport operations. Green bars represent Neste's LCA values from used cooking oil sourced in Indonesia, USA, China, and Germany.

Figure 8 shows the total embodied SAF greenhouse gas emissions shown in Table 6, compared to Neste's calculations. Here, a difference in feedstock procurement is observed due to shipping of feedstock from each country to Finland. With energy-based allocation methods TCD calculate a 23.23 gCO_2e/MJ compared to 7.51 gCO_2e/MJ from Neste for used cooking oil SAF from Indonesia. What's noticeable about Neste's values is that each Neste total LCA value is less than TCD's sole fuel production emissions. This is also true for literature and CORSIA values in Table 8 for all cases except USA used cooking oil total LCA emissions compared to CORSIA's sole fuel production emissions. The synopsis of literature in Table 3 in the literature review section of this report also shows higher total LCA values for used cooking oil SAF sourced from the USA. This shows ours and other LCA calculator methodologies is not a direct replication of Neste's production process, and improvements need to be made. The total TCD emissions must decrease by 68% to match Neste. It is therefore evident that there is a lack of information transferred between fuel production companies and LCA researchers, as no literature studies of the same fuel production process agree with Neste's low values. This study is not a complete partnership with Neste, but it is the beginning of more industry engagement to shorten that gap.

The results from feedstock production and procurement show that there is a small share of emissions arising from the activities of this stage (7.33 gCO_2e/MJ). This low result was expected as this scenario considered SAF made from 100% used cooking oil, classed as a waste material, and thus land-use-change emissions were avoided. If another feedstock was considered, such as vegetable oil from purpose grown feedstocks, the system boundary of this stage would include significantly more elements such as machinery emissions from feedstock production, fertilizer emissions and land use change. The airport operation activities had a minor effect on the total results, 1.5% of emissions from this section are from the auxiliary airport operations emissions. The aircraft results show that 2521.5 kg of fuel was used during the flight considered in this scenario.

The total greenhouse gas emissions that are embodied in the SAF were calculated by adding the emissions from each section studied. The LCA calculation returned a range of 16.56-24.85 gCO_2e/MJ_{SAF}. Compared to the Jet-A reference of 89 gCO_2e/MJ, this represents a reduction of up to 81%. Neste claims that their SAF offers greenhouse gas reduction of up to 80%, hence this LCA study is consistent with Neste's claims [64].

There are four options for feedstock sourcing revealed by Neste; they are used cooking oil from Germany, Indonesia, USA, and China. The difference in LCA value for these regions is shown below in Table 8, see the "Feedstock" row. The range in LCA values is important as it shows the impact of emissions associated from transportation of feedstock from different regions. These results combine to provide a range of values associated with Ryanair's SAF use.

Table 8: Total Embodied SAF greenhouse gas emissions from used cooking oil sourced from different regions, with revenue passenger kilometre conversion. This table combines the total emissions from the feedstock, fuel production, and airport operations element of TCD's LCA model, and combines them to give a total LCA value in both gCO_2e/MJ_{SAF} and gCO_2e/RPK. The calculated TCD values are then compared to Neste values [63, 64] and literature values from De Jong [39] and one of CORSIA's methodology values [13] from Table 1 for renewable jet fuel produced from used cooking oil.

Total Embodied SAF GHG Emissions	TCD Indonesia	TCD USA	TCD China	TCD Germany	De Jong	CORISA	Units
Feedstock	7.33	3.24	8.95	0.65	2.4	3.9	gCO_2e/MJ_{SAF}
Fuel Production	15.31	15.31	15.31	15.31	23.7	10.5	gCO_2e/MJ_{SAF}
Airport Operations	0.60	0.60	0.60	0.60	1.27	0.5	gCO_2e/MJ_{SAF}
Total	23.23	19.15	24.85	16.56	27.37	14.8	gCO_2e/MJ_{SAF}
NESTE Comparison	7.51	11.08	10.22	7.21	7.21-11.08	7.21-11.08	gCO_2e/MJ_{SAF}
Total LCA emissions in gCO_2e/RPK from Ryanair Scenario 1 aircraft assumptions							
100% Jet-A	68.69	68.69	68.69	68.69	68.69	68.69	gCO2e/RPK
40% SAF, 60% Jet-A	48.47	47.20	48.98	46.39	49.77	45.85	gCO2e/RPK
100% SAF	18.17	14.99	19.43	12.97	21.37	11.58	gCO2e/RPK

Table 8 compares the TCD results for the different regions compared to literature and CORSIA values. Note here that the TCD LCA methodology concerning airport operations considers many aspects of airport logistics while the literature and CORSIA values contain the transport and distribution of the hydroprocessed renewable jet fuel to the airport only. TCD's LCA results were lower than De Jong [39] and higher than CORSIA [13] for the same parameters. For fuel production, De Jong is 54% higher than TCD's value, and CORSIA is 31% lower than TCD's value. GREET was used in both other studies to model fuel production emissions. The inconsistency in these values using the same model shows the need for a more reliable scientific approach to fuel production emissions modelling, rather than an input-based methodology that is observed in GREET. This modelling approach can be used and adapted by

existing LCA calculators like GREET, GHGenius, and BioGrace to improve their fuel production emissions calculation.

If a 100% SAF blend was used, the total LCA greenhouse gas emissions for this scenario would be in the range of 12.97-18.17 gCO_2e/RPK. This is very low compared to current industry levels, for example; Ryanair's pre-Covid value was 66 gCO_2/RPK [62] and Lufthansa's pre-Covid value was 92.2 gCO_2/RPK. When the emissions were calculated for this scenario with 100% Jet-A fuel, the result was 68.69 gCO_2e/RPK. This is very close to Ryanair's current level and serves as a point of validation. The expected use case of a 40% blend is then assessed. The result of this is a range of 46.39-48.98 gCO_2e/RPK. Ryanair has a goal of 60 gCO_2/RPK by 2030. This shows that Ryanair's SAF use and operational emissions in this scenario are within this goal and will help Ryanair decarbonize.

Section 3.1 shows the chemical reactions used in the fuel production model to measure the change in mass throughout the production process. The modelled reactions assume the fuel is converted to 100% alkanes. This is an assumption that aims to reduce calculation complexity, as hydroprocessed renewable jet fuel is not 100% alkanes. It is assumed here that the formation of iso-alkanes, cycloalkanes, and other molecules present in hydroprocessed renewable jet fuel follow a similar reaction pathway or are produced from these alkanes. Currently, the methods used provide a meaningful calculation for Ryanair Scenario 1 but can be improved for Ryanair Scenario 2.

6. Conclusions

The LCA methodology discussed in this project describes the fuel production element of Ryanair Scenario 1. The fuel production model described in this report tracks the molecular changes in the used cooking oil feedstock in its conversion to hydroprocessed renewable jet fuel SAF. Using the physical properties of the molecules, the reaction mechanism in the conversion of used cooking oil to SAF, TCD assumptions, and industry information, the emissions to relating to fuel production can be better estimated rather than existing LCA calculators that rely on accurate user-inputs. A key finding though literature and LCA calculator research is that this methodology of calculating fuel production emissions is unique and is not present in current LCA literature. The total LCA methodology is also unique, as it considers aspects in LCA that are specific to Ryanair and is a complete representation of their operations. This industrial partnership allows for better, more accurate research in life cycle

assessment, and does not rely on generalised assumptions and accurate user-inputs like current LCA calculators [14, 21, 22, 28] and calculator users such as CORSIA [13].

This is a gap in LCA tools that can be filled. No current LCA tool or literature use a mass balance and reaction kinetics approach to estimate life cycle emissions and specific inputs for sustainable aviation fuel production. The TCD fuel production model uses this approach to estimate the emissions and specific inputs required for used cooking oil derived hydroprocessed renewable jet fuel. The physical properties of the molecules present in the reaction mechanism are used to determine the energy use in conversion, and the mass balance in the reaction mechanism calculates the specific hydrogen needed for conversion of used cooking oil into sustainable aviation fuel, and calculated the intrinsic CO_2 produced in the production process. This model can be customised and adapted to incorporate renewable hydrogen use, renewable electricity production, and assess other vegetable oil feedstocks to estimate the GHG emissions of SAF production though their triglyceride compositions.

This research provides a final LCA value for the production of Neste's [64] sustainable aviation fuel. This result combines with other research in the Ryanair Sustainable Aviation Research Centre to analyse the use of Neste's SAF by the operations defined in Ryanair Scenario 1. Through the four areas of Feedstock, Fuel Production, Airport, and Aircraft, it was found that the use of Neste SAF in Ryanair's Boeing 737-8200 from Amsterdam Schiphol Airport to Dublin Airport yielded a greenhouse gas LCA range of 16.56-24.85 gCO_2e/MJ_{SAF} or 12.97-18.17 gCO2e/RPK using 100% SAF. This analysis shows a potential for Ryanair to decrease emissions by up to 81%. With Ryanair's aim to increase use of this SAF to a blending fraction of 40%, this becomes 60.02-63.34 gCO_2e/MJ_{SAF} or 46.39-48.98 gCO2e/RPK, which will contribute to their goal to cut their emissions to under 60 gCO2e/RPK by 2030, leading to a decrease in emissions by up to 32% compared to 100% Jet-A. This analysis will assist in Ryanair's emission reduction strategy, while contributing to the much-needed research in LCA.

7. Future Work

The plan for the immediate future is to report the findings of the TCD fuel production model in a scientific paper. I am currently in the process of writing this paper, it is described under "Paper 1" below. Secondly, I am assisting my colleague in their reporting of the TCD LCA methodology to Gold Standard [65] for third party verification. This methodology is being presented at ACS Spring 2023 and will result in a second author publication. It is described under "Paper 3". My second first author publication will be another aspect of fuel production

modelling, however a different production pathway. For this publication, I will focus on Ethanol-to-Jet (ETJ) which is an upcoming form of sustainable aviation fuel. This is described under "Paper 2".

Paper 1: A reaction kinetics approach fuel production emissions modelling of used cooking oil (UCO) derived hydroprocessed renewable jet (HRJ) sustainable aviation fuel (SAF).

Lead Author: Liam Mannion.

Second Authors: Aron Bell, Mohammad Reza Ghaani, Stephen Dooley.

For this paper, I will focus on the fuel production element of LCA. This paper will describe the methodology of the fuel production model from Ryanair Scenario 1 and have a comparison to existing LCA tools. I will provide a description of the TCD fuel production methodology, reaction mechanism, mass and energy balance, energy involved in conversion from reactants to products and co-products, equations used in the model, and energy use calculations for each step in the fuel production process. The focus of this paper is to highlight the valuable inputs such as hydrogen use and production parameters can be modelled internally rather than relying on the user. This is something that is new to current LCA literatre, as no current LCA tool uses a mass and energy balance approach to calculating sustainable aviation fuel emissions. I also want to create an array of possible results depending on factors such as: co-product allocation methods, country of facility, efficiency of overall facility, explore e-SAF and effect of fossil fuel vs renewable energy to fuel the facility. From this, I can compare the total energy in fuel production to other literature that calculates the fuel production emissions of used cooking oil hydroprocessed renewable jet fuel. The expected conclusion of this paper is that current LCA calculators are too user reliant for important inputs that can be derived from studying the elemental flow of the molecules throughout the production steps, the reaction mechanism for the conversion of used cooking oil triglycerides to sustainable aviation fuel, and how this model has the potential then to be adopted by other LCA calculators and improve their LCA calculation methodology.

Paper 2: A reaction kinetics approach fuel production emissions modelling of agricultural and forestry waste derived ethanol-to-jet (ETJ) sustainable aviation fuel (SAF).

Lead Author: Liam Mannion.

Second Authors: Aron Bell, Mohammad Reza Ghaani, Stephen Dooley.

For my second first author paper, I plan to build a new model that focuses on the conversion of ethanol to jet fuel. Ethanol-to-jet is an up in coming method of sustainable aviation fuel production that focuses on waste products such as forest and agricultural residues to make renewable ethanol to be upgraded to jet fuel in high pressure reaction chambers. The expected conclusion of this paper is that ethanol-to-jet fuel is very energy intensive and is heavily reliant on a limited waste feedstock.

Paper 3: Life cycle assessment of European airlines operation scenarios using specific hydrotreated renewable jet fuel derived from used cooking oil

Lead Author: Aron Bell.

Second Authors: Liam Mannion, Tiarnán Murphy, Mark Kelly, Mohammad Reza Ghaani, Stephen Dooley

Life cycle assessment (LCA) calculations of greenhouse gases (GHGs) per revenue passenger kilometre for Ryanair flights under various scenarios are evaluated. Current state of art tends to focus solely on the LCA of the fuel; however, this work considers the entire lifecycle of flight operations and hence, gCO2e/RPK (grammes of CO2 equivalent per revenue passenger-kilometre) is the functional unit. Key parameters such as flight route, blend of hydrotreated renewable jet fuel (HRJ) and HRJ supply chain are assessed to understand the impact of each on the carbon intensity of the overall aviation activity.

The lifecycle of the HRJ and flight operations are broken into four sections: Feedstock Production and Procurement, Fuel Production, Airport Operations and Aircraft Operations. Feedstock Production and Procurement analyzes all activity involved with transporting the used cooking oil feedstock prior to the fuel production steps. Fuel Production includes all activity involved in the conversion of the feedstock into HRJ. Airport Operations includes all activity involved in transporting the HRJ from the refinery to the aircraft and the auxiliary activity necessary for the flight operation. Aircraft Operations determines the quantity and quality of fuel conversion due to the flight and uses logged flight data on a specific basis. In instances where specific data cannot be provided by external stakeholders, assumptions are made from the scientific literature and/or physical science relations to calculate the total GHGs from activities within the system boundary.

This work emphasises supply chain analysis particular to the specific aviation activity studied. It is found that existing LCA tools have limited compatibility with this paradigm as

they do not allow full control or transparency over the mathematics behind the model. So as not to be constrained by existing assumptions or system boundaries, calculations are performed by hand, following rigorous physical science relations, and emphasising the use of data of the actual supply chain studied. Comparisons are made to equivalent results from existing LCA tools such as GREET and GHGenius. Key findings show that parameters such as location of HRJ feedstock procurement, mode of fuel transportation, and the carbon intensity of electricity generation, have a significant effect on the GHG emissions from the aviation activity and hence the specific flight emissions per revenue passenger-kilometre.

Non-publication future work:

I will also work with Aron Bell, Dr. Stephen Dooley, Mohammad Reza Ghaani, and Mark Kelly to develop Ryanair Scenario #2, #3 and #4. Taking one at a time, I will assess useful criteria (destinations, SAF supplier, airports) that correspond to industry needs in emissions assessment with my colleagues at the Ryanair Sustainable Aviation Research Centre. In the meantime, some immediate work that can be applied to the fuel production model are the following:

1. Development of alternative feedstock pathways, e.g., Tallow, Rapeseed oil, Soybean Oil, algae, and multiple feedstocks.
2. Effect of renewable on-site hydrogen production from renewable hydrolysis.

The points above are reliant on the result from Ryanair Scenario 1, hence the best action forward is to focus on the completion and certification to Gold Standard of the Ryanair Scenario 1 methodology, then focus on publications. Figure 9 shows a timeline of my future work to 2025.
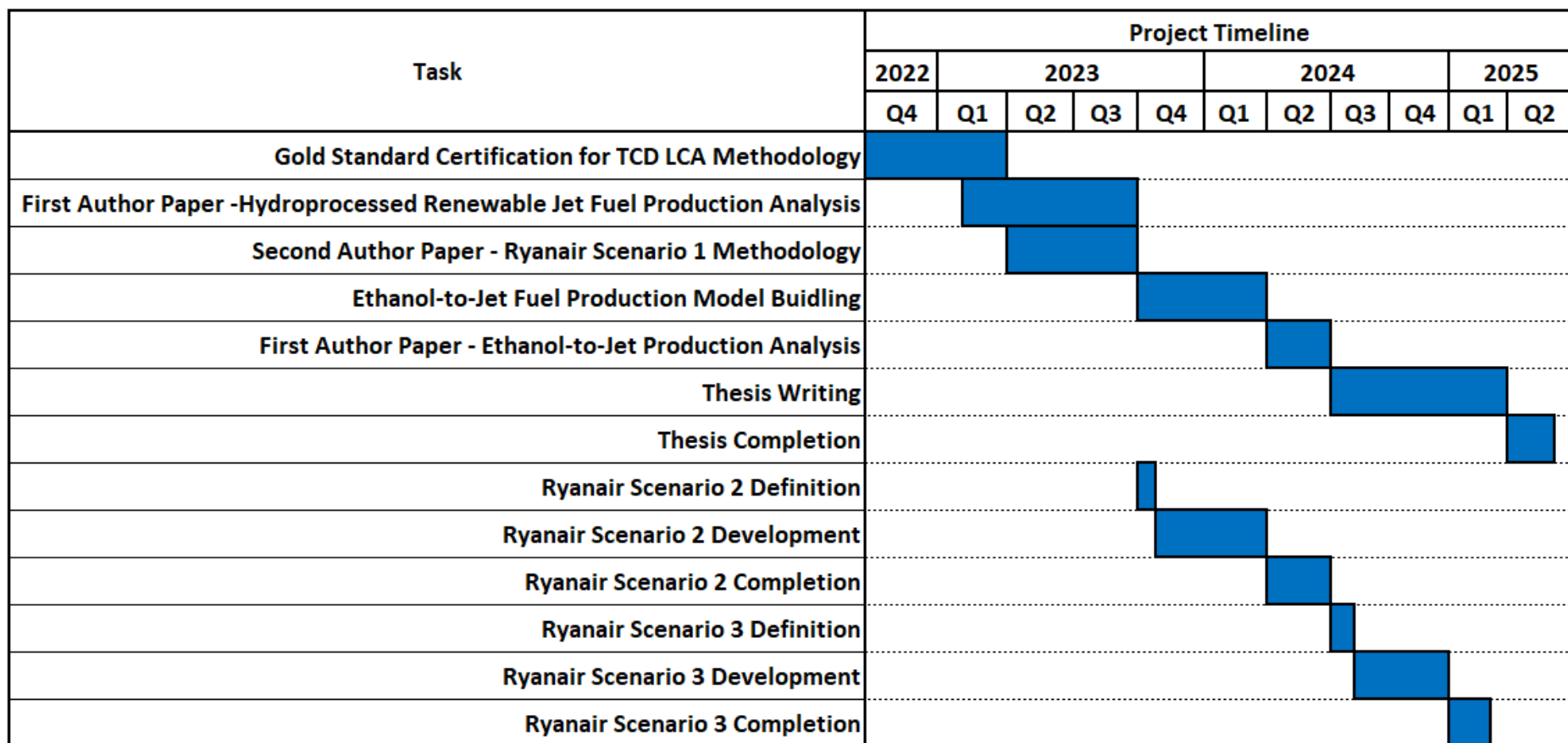
Task	Project Timeline										
	2022	2023				2024				2025	
	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2
Gold Standard Certification for TCD LCA Methodology	■	■									
First Author Paper -Hydroprocessed Renewable Jet Fuel Production Analysis		■	■	■							
Second Author Paper - Ryanair Scenario 1 Methodology			■	■							
Ethanol-to-Jet Fuel Production Model Buidling					■	■					
First Author Paper - Ethanol-to-Jet Production Analysis							■				
Thesis Writing								■	■	■	
Thesis Completion											■
Ryanair Scenario 2 Definition					■						
Ryanair Scenario 2 Development						■	■				
Ryanair Scenario 2 Completion							■	■			
Ryanair Scenario 3 Definition									■		
Ryanair Scenario 3 Development									■	■	
Ryanair Scenario 3 Completion										■	

Figure 9: Gantt chart of research and work strategy for Liam Mannion from 2022-2025

List of Publications and Presentations

[1]. L. Mannion, S. Dooley. "Life cycle assessment of sustainable aviation fuel and sensitivity analysis of feedstock farming emissions using GREET". MaREI Symposium. Poster Presentation. National University of Ireland Galway. 27/05/22.

[2]. L. Mannion, A. Bell, S. Dooley. "Life cycle assessment of Ryanair operations using sustainable aviation fuel". Ryanair Sustainability Day 2022 – Pathway to Net Zero. Poster Presentation. Trinity College Dublin. 01/12/22.

[3]. A. Bell, L. Mannion, S. Dooley. "Life cycle assessment of European airlines operation scenarios using specific hydrotreated renewable jet fuel derived from used cooking oil". ACS Spring 2023. Oral Presentation. 26/3/23.

[4]. A. Bell, L. Mannion, S. Dooley. "Life cycle assessment of European airlines operation scenarios using specific hydrotreated renewable jet fuel derived from used cooking oil". ACS Spring 2023. Poster Presentation. 28/3/23.

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Appendix

1. Assumptions in Feedstock Production Model

[FP1]   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.

[FP2]   Chemical reactions are 100% converted in the forward reaction rate for the full reaction mechanism, as given by the yields reported in [51], unless stated otherwise.

[FP3]   The energy produced due to losses of heat, and maintaining the fuel constant temperature I conatained within the system efficency parameter. More information is needed.

[FP4]   The SAF energy density is set to be in the range of the ASTM 7566 Standard minimum and reported LHV for UOP hydroprocessed renewable jet fuel of 42.8-43.9 MJ/kg.

[FP5]   The fuel production facilty is assumed to be in Finland, with electricity from the main grid as source. This emission factor associated with electricity utilisation uses an average greenhouse gas intensity based on Finlands electricity production facilities from [47] (mix of renewables and fossil fuels).

[FP6]   Fuel production is assumed to use 100% electricity as energy source. 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.

[FP7]   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.

[FP8]   The used cooking oil is assumed to have a compostion of 79.1% triglycerides, 1.8% diglcerides,2.2 % monoglycerides, and 16.9% free fatty acids. Of the triglcerides, the composition is assumed to be 32.8% triolein, 6.5% tripalmitin, and 60% trilinolein.

[FP9]   For hydrogenation, it is assumed that hydrogen is added in excess by a factor of ~35% of the mass needed to perform the hydrogenation.

[FP10] The initial feedstock is heated from to 400 C from 25 C. in the hydrocracking bath. (Based on the range of 350-450 C from literature) [51]

[FP11] 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.

[FP12] Hydrocracking occurs at 400 C and takes place for 4 hours.

[FP13] Only propane is removed at the propane cleave step. This is not evidenced.

[FP14] Propane cleave occurs at 400 C for 1 hour.

[FP15] Deoxygenation/Decarbonization occurs at 400 C for 4 hours.

[FP16] CO2 produced in the reaction process is captured directly from bath. It still contributes to the overall CO2 cost.

[FP17] Vapour-liquid separation occurs at 400 C for 1 hour.

[FP18] Propane is purified using numbers for Naphtha purification. This is not evidenced.

[FP19] Propane purification occurs at 400 C for 1 hour.

[FP20] Second hydrocracking occurs at 400 C for 4 hours.

[FP21] Fractional distillation 1 occurs at 350 C for 4 hours.

[FP22] Fractional distillation 2 occurs at 350 C for 4 hours.

[FP23] Naphtha, propane, and other gases are separated and purified maintaining heat and not cooling. More information is needed. This is not evidenced.

[FP24] Naphtha purification occurs at 400 C for 1 hour.

[FP25] Hydrogen used in fuel production is produced through steam methane reforming (SMR) which contributes its own intrinsic CO2 cost. More information is neeeded. This is not evidenced.

General FP Assumptions

[FP26] The fuel production system is a batch production method. This is not evidenced.

[FP27] There are no mass losses or residues left over in each reaction chamber. All elemental mass is conserved. This is not evidenced.

Reaction Mechanism Assumptions

[FP28] All chemical reactions are assumed to occur in one vessel, in a batch configuration accoridng to the reaction mechanism given in FuelProd5.

[FP29] Unknown triglcerides, diglycerides, and monoglycerides in fuel mixture are converted to analagous forms of carboxylic acids and follow the analagorous reaction mechanism.

[FP30] As unknown liquid phase products are produced, their gaseous co-product gas comprise only propane, water, CO & CO2 as defined in the reaction mechanism.

[FP31] For these "known unknowns", the proportions of known propane, water, and other gas yields are used and applied to the "known unknowns". More information is needed.

[FP32] Reaction mechanism is not specified on the basis of structural isomers, it is simplified by describin only normal alkane products, knowing that any structural isomers will follow the same mass flow. Hence the final composition of jet fuel hydroprocessed renewable jet fuel is modelled as 100% normal alkanes. This is not evidenced.

[FP33] 85% of the oleic acid acid is converted to stearic acid, 15% remains as oleic acid, as is defined by [51].

[FP34] Consumption of stearic, oleic, and palmitic acid is assumed to occur by three processes (Decarbonization, Decarbonylation, Hydrodeoxidation) at equal rates (ie. 0.33/0.33/0.33 by mass).

[FP35] Molecular cracking was manipulated to ensure the fuel mix contains a distribution of alkanes representative of Jet-A fuel. The distribution was made to represent a GC x GC analysis by J. Heynes [70]. The cracking proportions are shown in the supplementary materials.

Mass Flow Equations Assumptions

[FP36] Energy calculation for hydrotreatment is calculated on specific heat capacity of heating known mass of triolein, trilinolein, and tripalmitin from 25-400 C. The reactions are mostly exothermic, hence any other energy required for the reactions to occur is taken internally.

Supplementary Materials

TCD LCA Tool:

https://docs.google.com/spreadsheets/d/10gOte3BoQRBbj8qF4cD9RsiuvKYsK_SK/edit?usp=sharing&ouid=107535767721949402461&rtpof=true&sd=true

Fuel production detailed reaction mechanism:

Step 1	1	Used Cooking Oil to fatty acids.	C57H104O6 + 3H2 → C3H8 + 3C18H34O2	Triolein + Hydrogen → Propane + Oleic acid
	2	Used Cooking Oil to fatty acids.	C57H98O6 + 3H2 → C3H8 + 3C18H32O2	Trilinolein + Hydrogen → Propane + Linoleic acid
	3	Used Cooking Oil to fatty acids.	C51H98O6 + 3H2 → C3H8 + 3C16H32O2	Tripalmitin + Hydrogen → Propane + Palmitic acid
Step 2	4	Fatty acid **hydrogenation** to	C18H34O2 + H2 → C18H36O2	Oleic acid + Hydrogen → Stearic acid

		saturated fatty acid (100%).		
	5	Fatty acid **hydrogenation** to saturated fatty acid (15%).	C18H32O2 + 2H2 → C18H36O2	Linoleic acid + Hydrogen → Stearic acid
Step 3	6	Saturated fatty acid **decarboxylation** to (normal) alkanes.	C18H36O2 → C17H36 + CO2	Stearic acid → Heptadecane + Carbon Dioxide
	7	Fatty acid **decarboxylation** to (normal) alkenes.	C18H34O2 → C17H34 + CO2	Oleic acid → Heptadecene + Carbon Dioxide
	8	Saturated fatty acid **decarboxylation** to (normal) alkanes.	C16H32O2 → C15H32 + CO2	Palmitic acid → Pentadecane + Carbon Dioxide
	9	Saturated fatty acid **decarbonylation** to (normal) alkanes.	C18H36O2 + H2 → C17H36 + CO + H2O	Stearic acid + Hydrogen → Hepadecane + Carbon monoxide + Water
	10	Fatty acid **decarbonylation** to (normal) alkenes.	C18H34O2 + H2 → C17H34 + CO + H2O	Oleic acid + Hydrogen → Heptadecene + Carbon monoxide + Water
	11	Saturated fatty acid **decarbonylation** to (normal) alkanes.	C16H32O2 + H2 → C15H32 + CO + H2O	Palmitic acid + Hydrogen → Pentadecane + Carbon monoxide + Water
	12	Saturated fatty acid **hydrodeoxygenation** to (normal) alkanes.	C18H36O2 + 3H2 → C18H38 + 2H2O	Stearic acid + Hydrogen → Octadecane + Water
	13	Fatty acid **hydrodeoxygenation** to (normal) alkenes.	C18H34O2 + 3H2 → C18H36 + 2H2O	Oleic acid + Hydrogen → Octadecene + Water
	14	Saturated fatty acid **hydrodeoxygenation** to (normal) alkanes.	C16H32O2 + 3H2 → C16H34 + 2H2O	Palmitic acid + Hydrogen → Hexadecane + Water
Step 4	15	Alkenes **hydrogenation** to alkanes.	C17H34 + H2 → C17H36	Heptadecene + Hydrogen → Heptadecane
	16	Alkenes **hydrogenation** to alkanes.	C18H36 + H2 → C18H38	Octadecene + Hydrogen → Octadecane
Step 5	17	**Cracking** of octadecane.	C18H38 + 0.9H2 → 0.1C18H38 + 0.9(C10H22 + C8H18)	Octadecane + Hydrogen → Octadecane + Decane + Octane
	18	**Cracking** of heptadecane.	C17H36 + H2 → 0.08C17H38 + 0.29(C11H24 + C6H14) + 0.23(C8H18 + C9H20) + 0.17(C13H28 + C4H10) + 0.23(C12H26+C5H12)	Heptadecane + Hydrogen → Heptadecane + Unedecane + Hexane + Ocatane + Nonane + Triecane + Butane + Dodecane + Pentane
	19	**Cracking** of hexadecane.	C16H34 + 0.9H2 → 0.1C16H34 + 0.9(C9H20 + C7H16)	Hexadecane + Hydrogen → Hexadecane + Nonane + Heptane
	20	**Cracking** of pentadecane.	C15H32 + 2/3H2 → 1/3C15H32 + 2/3(C9H20 + C6H14)	Pentadecane + Hydrogen → Pentane + Nonane + Hexane
	21	**Cracking** of unknown paraffins.	CxHy + 1.1375H2 → 0.2125(C11H24) + 0.175(C12H26) + 0.0875(C13H28) + 0.3125(C14H30) + 0.2125(C15H32)	n-Paraffins + Hydrogen → Undecane + Dodecane + Tridecane + Tetradecane + Pentadecane
	22	**Cracking** of octane.	C8H18 + 0.5H2 → 0.5(C8H18) + 0.5(2C4H10)	Octadecane → Octadecane + Decane + Octane