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Comparative Life Cycle Assessment of Sustainable Aviation Fuels: Country-based study of Alcohol-to-Jet Pathways at the European level

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Preface

This master's thesis was carried out in the Department of Energy and Process Engineering at the Norwegian University of Science and Technology (NTNU) in Trondheim, from August 2023 until January 2024, as part of the Erasmus+ exchange program between the University of Padua and NTNU. The research project was conducted under the supervision of Prof. Francesco Cherubini, Prof. Marcos Djun Barbosa Watanabe and Prof. Anna Stoppato , within the framework of the Industrial Ecological Program (IndEcol). The aim of IndEcol is to address the preservation of ecosystem services, biodiversity, and climate regulation in response to rising societal demands for bioenergy, food, and biomaterials.

Abstract

The aviation industry, responsible for 2% of anthropogenic emissions, faces the challenge of achieving net zero emissions by 2050. The International Civil Aviation Organization (ICAO) highlights the importance of supporting technological and operational advances in the coming years, identifying Sustainable Aviation Fuels (SAFs) as a crucial solution. Regulatory initiatives, exemplified by the European Commission's Fit for 55 program and ReFuel EU Aviation initiative, aim to increase the presence of SAFs at EU airports, in line with broader emissions reduction goals. Although they currently make up less than 0.1% of aviation fuels, SAFs, particularly drop-in variants, are expected to rise to 6% by 2030, with a long-term goal of reaching 70% by 2050 in Europe.

This thesis conducts a comparative life cycle assessment (LCA) to examine the environmental impacts of SAFs derived from alcohol-to-jet (ATJ) pathways. Focusing on lignocellulosic biomass in the European context, the study analyzes six "well-to-wings" scenarios, that is, from biomass farming to fuel combustion. These scenarios differ in terms of the lignocellulosic biomass chosen (e.g., herbaceous energy crops, residues) and chemical intermediates (e.g., ethanol, isobutanol, or isobutene) derived from the respective fermentation processes and subsequently converted to SAF. Using a country-specific approach, the research clarifies regional variations in the environmental performance of alcohol-jet pathways, providing insights into their suitability for sustainable aviation in the European sector. Additionally, the study aimed to assess the scalability of these technologies within the European context, examining the potential for country-specific SAF production to meet jet fuel demand and evaluating the climate change mitigation potential resulting from SAF utilization in aircraft. This study contributes to the ongoing discourse on environmentally friendly alternatives to conventional jet fuels, responding to the imperative for sustainable practices in the aviation industry.

Riassunto

L'industria dell'aviazione, responsabile del 2% delle emissioni antropiche, deve affrontare la sfida di raggiungere emissioni nette zero entro il 2050. L'Organizzazione Internazionale dell'Aviazione Civile (ICAO) sottolinea l'importanza di sostenere i progressi tecnologici e operativi nei prossimi anni, individuando nei carburanti sostenibili per l'aviazione (SAF) una soluzione cruciale. Le iniziative normative, come il programma Fit for 55 della Commissione europea e l'iniziativa ReFuel EU Aviation, mirano ad aumentare la presenza dei SAF negli aeroporti dell'UE, in linea con gli obiettivi più ampi di riduzione delle emissioni. Sebbene attualmente costituiscano meno dello 0,1% dei carburanti per l'aviazione, si prevede che i SAF, in particolare le varianti drop-in, salgano al 6% entro il 2030, con l'obiettivo a lungo termine di raggiungere il 70% entro il 2050 in Europa.

Questa tesi conduce un'analisi comparativa del ciclo di vita (LCA) per esaminare gli impatti ambientali dei SAF derivati da filiere di produzione "alcohol-to-jet" (ATJ). Concentrandosi sulla biomassa lignocellulosica nel contesto europeo, lo studio analizza sei scenari "well-to-wings", ovvero dalla coltivazione della biomassa alla combustione del carburante. Questi scenari differiscono in termini di biomassa lignocellulosica scelta (ad esempio, colture energetiche erbacee, residui) e intermedi chimici (ad esempio, etanolo, isobutanolo o isobutene) derivati dai rispettivi processi di fermentazione e successivamente convertiti in SAF. Utilizzando un approccio specifico per ogni Paese, la ricerca chiarisce le variazioni regionali nelle prestazioni ambientali dei percorsi alcool-jet, fornendo indicazioni sulla loro idoneità per un'aviazione sostenibile nel settore europeo. Inoltre, lo studio mira a valutare la scalabilità di queste tecnologie nel contesto europeo, esaminando il potenziale di produzione di SAF specifico per ogni Paese per soddisfare la domanda di carburante per aerei e valutando il potenziale di mitigazione del cambiamento climatico derivante dall'utilizzo di SAF negli aerei. Questo studio contribuisce al dibattito in corso sulle alternative ecologiche ai carburanti per jet convenzionali, rispondendo all'imperativo di garantire pratiche sostenibili nell'industria dell'aviazione.

Acknowledgments

"…and then he took a plane to Norway"

With this thesis, a long journey is coming to an end, and not even landing can quell the dizziness of what I experienced.

The years at the University of Padua, complemented by two thrilling Erasmus adventures in Brno and Trondheim, represents an essential junction in the formation of the person I am now and will one day become. This experience allowed me to broaden my horizons to territories to which my eyes were not accustomed, to cultivate relationships for which my heart did not know it had room, and to discover new and challenging ways of thinking. These have been intense years in every way, but without a doubt what will remain most will be the people with whom I had the honor of sharing the trip.

I would like to thank everyone who came across my passage during this period, even with the people with whom I shared only a few hours, scattered among the corners of Europe and of whom, due to the fleeting moment combined with the effect of a crappy vodka, nothing remains but an anonymous blurred memory.

One can be a good traveling companion even just for one night.

After that I thank professors who have succeeded each other over the years from those who have left a mark of respect and admiration to those who have made me conjure up all the saints of the Academic Calendar. In particular I would like to thank Prof. Anna Stoppato and Professor Marcos Djun Barbosa Watanabe for their important contribution in the writing of this thesis.

Thanks to my two greatest vices on which I did my bachelor's thesis and master's thesis, respectively: Marijuana and alcohol. I would say that you have given me more than you have taken away.

Finally, a few words are in order for all those who are an intimate and profound presence in my life.

Thank you to all my friends, Brotherhood, Bordanhood, Masci, my scout group and my Erasmus friends scattered all over the world, you are what spurs me the most to bring out the best and worst in me. You are an endless spring of happiness.

Finally, thank you to my family for your support and patience, gratuitous and genuine dedication to me, if ever in my life I should have merits these would be largely shared with you. I love you.

I dedicate this thesis to the memory of my grandmother Armida Bedin (1926-2023).

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Nomenclature

ICAO	International Civil Aviation Organization
SAF	Sustainable Aviation Fuel
LCA	Life cycle assessment
ATJ	Alcohol-to-Jet
COVID 19	COronaVIrus Disease 19
IEA	International Energy Agency
NZE	Net Zero Emissions
LTAG	Long-Term global Aspirational Goal
ATM	Air Traffic Management
LCAF	Low Carbon Aviation Fuel
ANSP	Air Navigation Service Provider
CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
RED	Renewable Energy Directive
GHG	Greenhouse Gases
DLUC	Direct Land Use Changes
ILUC	Inirect Land Use Changes
FT	Fischer-Tropsch
HEFA	Hydroprocessed Esters and Fatty Acids
SIP	Synthesized Iso-Paraffinic kerosene
CH	Catalytic Hydrothermolysis
HC-HEFA	Hydroprocessed Hydrocarbons, Esters and Fatty Acids
PtL	Power-to-Liquid
TRL	Technology Readiness Levels
ASTM	American Society for Testing and Materials

BETO	Department of Energy's Bioenergy Technologies Office
EIA	Energy Information Agency
EtOH	Ethanol
i-BuOH	Isobutanol
IBN	Isobutene
GB	Global Bioenergies
SSF	Simultaneous saccharification and fermentation
CHP	Combined Heat and Power
IPCC	Intergovernmental Panel on Climate Change
GWP	Global Warming Potential
GWP100	Global Warming Potential over 100 years
ESA-CCI	European Space Agency Climate Change Initiative
GAEZ	Global Agro-Ecological Zones
TEA	Techno-Economic Analysis
MIT	Massachusetts Institute of Technology
ANL	Argonne National Laboratory (ANL)
NREL	National Renewable Energy Laboratory
LCI	Life Cycle Inventory
ETJ	Ethanol-to-Jet
REWOFUEL	REsidual soft WOod conversion to high characteristics drop-in bioFUELs
RWH	Residual softwood into Hydrolysate RWH
LI-CHP	Lignin-Cogeneration Heat and Power
EFSA	European Food Safety Authority
LHV	Lower Heating Value
STATFOR	Statistics and Forecast Service

EAN   European Air Network

ISO   International Organization for Standardization

LCIA   Life Cycle Impact Assessment

Introduction

In this chapter the motivation for this research on assessing the life cycle for Sustainable aviation fuel production will be presented, by introducing a survey of the aviation sectors and its future perspectives. The chapter subsequently outlines the objectives of the master's thesis project, and it concludes by providing an overview of its structure.

1.1 Motivation

Since the middle of the 20th century, the annual emissions of carbon dioxide derived from the combustion of fossil fuels, have always increased, jumping, from almost 11 billion tons of carbon dioxide per year in the 1960s to an estimated 36.6 billion tons in 2022 [1]. Because we emitted more into the atmosphere than the natural carbon cycle can absorb, it led to a consequential increase of the global carbon dioxide concentration in the atmosphere: if in the 1960s, the global growth rate of atmospheric carbon dioxide was roughly 0.8 ± 0.1 ppm per year, over few decades, the annual growth rate more than quadrupled. Consequently, the atmospheric concentration of carbon dioxide rose from 317 ppm to 417 ppm. [2]. The study of air bubbles trapped in mile-thick ice cores and other paleoclimate evidence, revealed that over the last 800,0000 years the Earth has never experienced such a high concentration of CO_2 and the previous highest peak, occurred through the last ice age cycles, was set to around 300 ppm. This means that the annual rate of increase in atmospheric carbon dioxide over the past 60 years is about 100 times faster than previous natural increases, such as those occurred at the end of the last ice age 11,000-17,000 years ago. [3] In fact, on the geologic time scale, the increase from the end of the last ice age to the present looks virtually instantaneous.

In this critical scenario, aviation sector accounts for 2% of global anthropogenic emissions [4], having grown faster than rail, road, or shipping transportations, over the last decades. In fact, the direct emissions from aviation fossil fuel combustion have increased on average by 2-3% since 1990, reaching its peak of 1000 Mt CO_2 in 2019. Due to the COVID-19 pandemic this value dropped to less than 600Mt CO_2 in 2020, but, as the restrictions eased, air passengers started to recover rapidly

in all regions except for China (due to the zero-COVID policy) and Russia (due to the war), setting a value of about 800Mt CO_2 in 2022. According to the International Energy Agency (IEA), without multiple measures in terms of policies, innovation and technologic deployment, acting to contain the growth, the emissions are expected to surpass their 2019 level around 2025 undermining the track towards the achievements of the Net Zero Emissions by 2050 (NZE) scenario for 2050.

During the 41st assembly of the International Civil Aviation Organization (ICAO) in October 2022, the 184 member states agreed on a collective long-term global aspirational goal (LTAG) of net zero carbon emissions from international aviation by 2050, in support of the Paris's agreement temperature goal [5]. The LTAG reports three possible scenarios (F1, F2, F3) of increasing level of ambitions considering technology, operations, and fuel. In each case, the results are shown for all three traffic forecasts (low, mid, and high) with prominence given to the mid traffic forecast.

The report states that innovation in air technology have the potential to reduce the CO_2 emissions by up to 21% in 2050, as outlined in the most demanding scenario. Advancements considered in the analysis comprise changes to current tube to wing aircraft, hybrid electric aircraft and exploration of new energy sources such as hydrogen and electricity. Clearly, evolution and revolution of the aircraft technology requires actions as soon as possible in terms of large-scale demonstration and investments together with increasing of availability of clean energy infrastructures.

Operation improvements have the potential to reduce the CO_2 emissions by up to 11% in 2050 that would be achieved by means of optimized route, enhanced ATM (Air traffic management), efficient and clean ground operation and formation flying.

Eventually ICAO appointed fuels as the key factor for the fulfillment of the targets since they offer the greatest potential to cut CO_2 emissions. Aviation fuel includes drop-in Sustainable Aviation Fuels (SAF), based on biomass, waste CO_2 streams and atmospheric CO_2 combined with hydrogen, lower carbon aviation fuels (LCAF), based on petroleum and non-drop-in fuels, such as hydrogen and

electricity. So far alternative propulsion options (i.e., electric driven and hybrid systems) and alternatives to jet fuel (e.g., liquid natural gas and hydrogen) have only been tested at the pilot-scale [6] [7] and there are still several technical issues associated with these alternatives [8]. Therefore, in the short-term evolution, aviation sector will require the use of drop-in sustainable aviation fuels (SAFs).

Drop-in SAFs neither require engine or system modifications in the aircraft, nor dedicated refueling infrastructure and, the emissions occurring during the combustion are offset by the CO_2 absorbed during the natural biomass growth, or the artificial CO_2 capture from concentrated waste streams or atmospheric sources. Nowadays, SAFs account for less than 0.1% of all aviation fuels consumed [4], while the demand for aviation fuel is dominated by jet kerosene. However, projections indicate a potential increase to 10% by 2030, in line with the Net Zero scenario. Beyond 2044, it is projected that SAF production could exceed aviation demand. By 2055, this shift is expected to lead to a significant reduction in fuel CO_2 emissions, up to 55% [9]. The largest contribution of this reduction would be given by SAFs derived from biomass (i.e., dedicated energy crops or agricultural and forestry residues), solid and liquid wastes, whereas the deployment of atmospheric CO_2 and hydrogen-based fuels is forecasted to take off in longer terms, after the second half of this century (F3 scenario). Keeping the focus on the Net Zero Scenario will require a significant ramp-up of investment in capacity to produce SAFs and supportive policies such as fuel taxes and low-carbon fuels standards. According to the mid-point scenario the worldwide amount of investment incurred by states, aircraft manufacturers, Air Navigation Service Providers (ANSPs), airports, airlines will be in the order 3500 billion dollars. [5]

Figure 1.1: CO2 Emissions Results - Integrated scenario F2 (Mid GHG reduction from Fuels) [5]

† Caution required with the interpretation of absolute CO_2 emissions levels after 2050 due to modelling assumptions e.g., frozen aircraft technology after 2050. Under these assumptions, CO_2 emissions are higher than in an alternative scenario (and modelling approach) where aircraft technology would continue to improve after 2050.
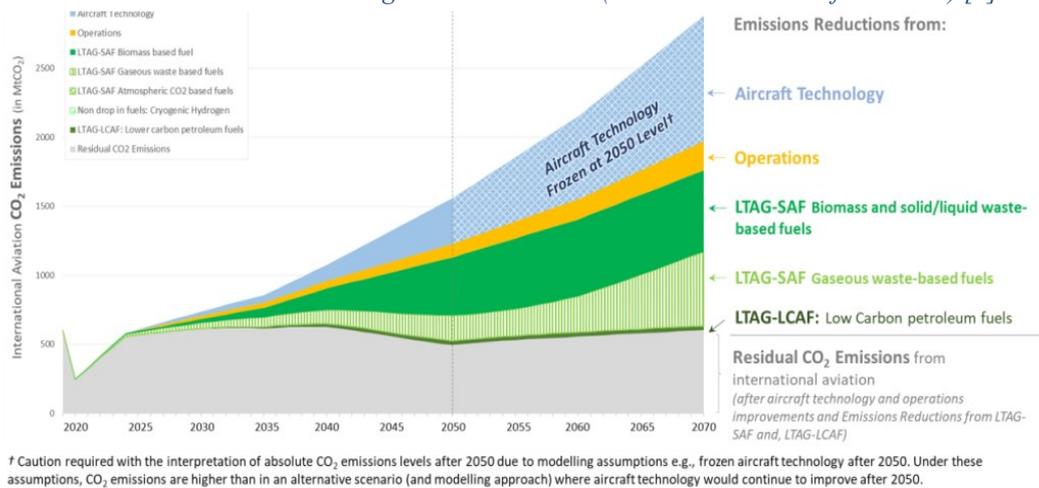
The 184 countries joining ICAO also agreed on a new baseline for the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) at 85% of the 2019 emissions level of international aviation, significantly more ambitious than the originally planned in 2016. Emissions beyond this would need to be reduced by purchasing certified emissions reductions to offset CO_2 emissions or by using sustainable aviation fuels. [10]

On July 14, 2021, the European Commission introduced the so called "Fit for 55", a package of proposals aims to reshape the way the EU deals climate, energy, land use, transport, and taxation to cut down on greenhouse gas emissions by at least 55% by 2030 compared to 1990 levels. The proposals include the RefuelEU Aviation Initiative, designed to enhance the environmental sustainability and fairness of air travel. [11]

Through this regulation, fuel suppliers are expected to adhere to new guidelines. They would gradually need to incorporate more advanced biofuels and synthetic aviation fuels (also known as e-fuels or renewable fuels of non-biological origin) at EU airports. The plan provides a timeline set in Annex I: 2% of the aviation fuel supplied should be sustainable by 2025, increasing to 6% by 2030, with a long-term goal of reaching 70% by 2050. There is also a specific rule for synthetic aviation fuels, starting at 1.2% in 2030 and gradually rising to 35% by 2050.

Additionally, the draft regulation imposes an obligation on aircraft operators to ensure that at least 90% of the yearly aviation fuel required is obtained at an EU airport. This measure is intended to curb fuel tankering practices, where planes are

intentionally over-fueled to avoid buying it at higher prices at another airport. The Commission sees this practice as harmful to the environment, as it adds weight to planes, increases fuel consumption, and raises emissions. Furthermore, it can create an uneven competition if some airlines benefit from lower fuel prices at their home base. The Commission emphasizes that planes leaving EU airports should be fueled precisely for the specific flight, while also adhering to safety rules.

To qualify as sustainable fuel, both ICAO CORSIA and RED II have established specific criteria [12]. For CORSIA eligibility, a fuel must meet sustainability standards, including life-cycle greenhouse gas (GHG) emissions at least 10% lower than the baseline of 89 gCO_{2eq}/MJ for petroleum jet fuel. Meanwhile, according to RED II the baseline is set to 94 gCO_{2eq}/MJ and the reduction percentages vary based on the installation date: at least 50% lower for installations predating October 5, 2015, 60% lower for those after that date, and 65% lower for biofuels produced in installations beginning operation after 2021.

Both the directives underscore the necessity for fuel not being made from biomass obtained from land with high carbon stock, respecting the areas of high importance for biodiversity, maintaining biodiversity and ecosystem services, contributing to local social and economic development and avoiding competition with food and water [13] [14]. These considerations are particularly relevant due to concerns about the impact of land use associated with specific aviation biofuels.

Direct land use changes (DLUC) occur when existing farmland is transformed to cultivate feedstock for biofuel production, while indirect land use changes (ILUC) happen as the growing demand for biofuels leads to land expansion, including the conversion of areas with high carbon stock such as forests, resulting in processes like deforestation and the release of CO_2 stored in trees and soil [15]. Studies indicate that converting land with substantial biodiversity, like rainforests or peatlands, can release several hundred times more CO_2-equivalent emissions than the subsequent biomass growth on that land can offset annually [16]. Consequently, biofuels derived from food and feed crops are not considered eligible under the ReFuelEU Aviation proposal due to these environmental concerns. Consequently, efforts are being made to investigate diverse feedstocks (i.e., lignocellulosic

biomasses) and production pathways that align more closely with the sustainable criteria established for SAFs [17]. This exploration aims to achieve significantly lower emissions compared to the conventional baseline, thereby contributing to a more environmentally responsible aviation industry.

Several pathways can be harnessed to produce Sustainable Aviation Fuel (SAF) using diverse feedstocks and supply chains. SAF pathways, including Hydroprocessed Esters and Fatty Acids (HEFA), Alcohols to Jet, Biomass Gasification + Fischer-Tropsch, and Power-to-Liquid (PtL), are anticipated to play a pivotal role in decarbonization in the short to medium term, remaining the primary contributors for long-haul flights in the long term [9].

HEFA-to-jet fuel pathway has been the most developed on commercial scale during the last decade [18] since adopted by big multinational companies such as Neste, that mainly rely on food wastes and residues for their feedstock portfolio and it currently produces around 90% of global SAF [19].

On the other hand, Alcohol-to-Jet (AtJ) pathways, characterized by one of the highest Technology Readiness Levels (TRL), have the capacity to produce SAF through the fermentation of processed lignocellulosic feedstocks. Exploring ATJ pathways could lead to valuable exploitation of agricultural and forestry residues, which in Europe amount to over 160 million tons per year [20], and herbaceous energy crops cultivated on abandoned lands, showing a potential production in Europe of around 100 million tons per year [21]. This approach significantly reduces direct and indirect land use changes, aligning with sustainability criteria defined by directives.

Additionally, some ATJ pathways offer the possibility of producing SAF that contains aromatics. While reducing aromatic content is beneficial for air quality and the environment, complete absence of aromatics in fuel may have airworthiness consequences for parts of the aircraft engine, such as rubber seals. This positions ATJ fuels as an option for future 100% SAF certification, surpassing today's blending limits.

Due to these considerations, as outlined by the ReFuelEU model, projections indicate that Alcohol-to-Jet (ATJ) Sustainable Aviation Fuel (SAF) supply is

anticipated to reach up to 5.8 million tons by 2050. This contribution is expected to represent approximately 20% of the total SAF supply in the EU27 [12].

1.2 Objective

Life Cycle Assessment (LCA) has been widely applied to evaluate the environmental impacts of energy production from agricultural and forest biomass residues and herbaceous energy crops [22] [23] [24]. However, there is a lack of research that evaluates the whole supply chain for SAF from renewable sources, in particular regarding second generation feedstocks in the European context. Hence, the objective of this thesis is to assess, by means of LCA analysis, the mass/energy balances and the environmental impacts of sustainable jet fuels produces from different lignocellulosic biomasses such as agricultural residues, forestry residues and herbaceous energy crops, mainly focusing on the European context. The assessment contemplates the life cycle "well-to-wings", via the alcohol-to-jet (ATJ) pathway, which entails ethanol, isobutanol as approved alcohols feedstocks for the upgrading process to SAFs [25] and isobutene as potential future chemical intermediate, which is still under consideration for inclusion as an additional annex to ASTM standard D7566 [26]. The goals that my thesis aims to attain are:

1) Assessing the supply chains of approved ATJ-based sustainable aviation fuels (i.e., ethanol and isobutanol) in the European context by using different feedstocks (i.e., residues and herbaceous energy crops).

2) Exploring the potential of isobutene as intermediate in the SAF supply chain.

3) Performing a comparison among the LCA-based climate impacts of different ATJ supply chains in terms of feedstocks and intermediates, highlighting the estimated emission reduction over against the conventional jet fuel baseline.

4) Estimating the climate change mitigation potential for utilizing those feedstocks to generate ATJ-based Sustainable Aviation Fuel (SAF) considering the European context.

1.3 Structure of the thesis

This thesis is structured as follows:

1. Introduction: provides an introduction to the research background motivation, objectives, and scope.

2. Literature review and theory: provides a research background on sustainable aviation fuels production, discussing approved pathways and focusing on the Alcohol-to-Jet (ATJ) conversion, along with analyzed feedstocks.

3. Method: presents the methodology adopted for simulating and assessing the life cycle of the selected pathways and therefore evaluating their environmental impacts.

4. Results and discussion: presents the simulation results and discusses them. Then draws conclusions regarding the effectiveness of the proposed pathways in comparison with baseline of conventional jet fuels (i.e., 100% fossil fuel based)

5. Conclusions: summarizes the key outcomes of this thesis, along with limitations of the study and recommendations for future work.

6. Appendix: provides additional calculations, results and supporting information related to the simulation models.

Literature review and theory

This chapter provides a theoretical background regarding the actual state-of-technology on sustainable aviation fuels production. First, a brief overview regarding all the possible approved pathways is presented and then the chapter focuses on a deeper description of the ATJ pathway and on the feedstocks includes in the analysis.

2.1 Aviation fuels

2.1.1 Conventional jet fuel

Conventional jet fuel, also referred as kerosene, is an aviation fuel designed specifically for commercial and military aircrafts. It is produced from the distillation of crude oil ranging from 205 °C to 260 °C in a process called atmospheric and vacuum fractional distillation accounting for around 10% of the crude oil cut, with gasoline and diesel making up the most of what remains. [27] According to a report from the Department of Energy's Bioenergy Technologies Office (BETO), out of one barrel of crude oil, around 15 liters are used to produce jet fuel and the worldwide aviation industry consumes approximately 1.5-1.7 billion barrels (178.6-202.4 billion liters) of conventional jet fuel per year [28].

The composition of jet fuel entails different compounds, such as hydrocarbons mainly ranging between C_8 and C_{16}, chemical components like alkanes, iso-alkanes, naphthenic or naphthenic derivatives and aromatic compounds [29]. The presence of each component directly affects the characteristic of the jet fuel, [30] for instance the high hydrogen-carbon ratio of alkanes increases the energy density of the fuel, while naphthenes help to reduce the freeze point, which is crucial for high-altitude flying. The presence of aromatics contributes to the lubricity to enhance the material compatibility and prevent leaks in the seals of some aircraft, but its content should be controlled in a reasonable range, since the excessive concentration might influence the cleanliness of the fuel. Besides the features above, commercial jet fuels must meet other strict requirements, including (1) maximum allowable deposits in standard heating tests, (2) maximum allowable viscosity, (3) maximum

allowable sulfur and aromatics content, (4) maximum allowable amount of wear in standardized test, (5) maximum acidity and mercaptan concentration, (6) minimum fuel electrical conductivity, and (7) minimum allowable flash point. [28] [30]

The most commonly used fuels for commercial aviation are called Jet A and Jet A-1. The ASTM D1655 establishes the standard specifications for traditional aviation turbine fuels. It sets the minimum property requirements for both Jet A and Jet A-1 aviation turbine fuels and provides a list of approved additives for use in civil engines and aircraft. Jet A, the standard jet fuel for both domestic and international flights, adheres to ASTM D1655 specifications, although it differs slightly from Jet A-1. The former is required to have a minimum flash point of 38°C and a freezing point not exceeding −40°C, whereas, Jet A-1 typically includes additional additives such as static dissipator, icing inhibitor, and antioxidant. Jet A-1 has a lower maximum freezing point of −47°C, making it suitable for long-haul international flights, particularly on polar routes during winter [31].

Some of the main property requirements of Jet A and Jet A-1 fuel complying with ASTM D1655 are presented in table 1.1.

Table 1.1: Jet A/Jet A-1 requirements specified by ASTM D1655 [31]

Fuel property	Jet A / Jet A-1	Test method (ASTM)
Composition		
Acidity, total mg KOH/g	≤0.10	D3242
Total aromatics, vol %	≤26.5	D6379
Sulfur, total mass%	≤0.3	D1266, D2622, D4294
Volatility		
Distillation range, °C		D86, D2887
10% recovery temperature	≤205	
Final boiling point °C	≤300	
Distillation residues, vol %	≤1.5	
Distillation loss, vol %	≤1.5	
Flash point, °C	≥38	D56, D3828
Density, 15°C kg/m^3	775-840	D1298, D4052
Mobility		
Freezing point, °C	≤-40 (Jet A)	D5972, D7153, D7154, D2386
	≤-47 (Jet A-1)	
Kinematic viscosity at -20°C, mm2/s	≤8	D445, D7042
Combustion		
Net heat of combustion, MJ/kg	≥42.8	D4529, D3338, D4809
Napthalenes, % vol	≤3	D1840
Thermal stability filter pressure drop at 260°C, mmHg	≤25	
Cleanliness		
Existent gum, mg/100ml	≤7	D381, D3948
Additive		
Antioxidant additive, mg/L	≤24	
Icing inhibitor additive range, vol%	0.07-0.15	

2.1.2 Sustainable aviation fuel

Despite their growing popularity, SAFs currently account for less than 0.1% of total aviation fuel demand [4]. Average global production of SAF from 2013 to 2015 was 0.29 million liters per year, rising to 6.45 million liters per year from 2016 to 2018, ranging between 240 and 380 thousand tons (300-450 million liters) in 2022 [32]. Global annual SAF production is projected to reach 6.5 Mt (8 billion liters) by 2032. As of 2021, only four companies, NESTE, Lanzatech, World Energy, and Gevo, are producing SAFs. However, numerous companies are investing in this emerging market, and several new production facilities have been announced in the United States, Europe, Asia, and South America to significantly increase SAF production in the long term [33].

Figure 1.1: Current and potential global SAF production capacity as of 2021 [33]
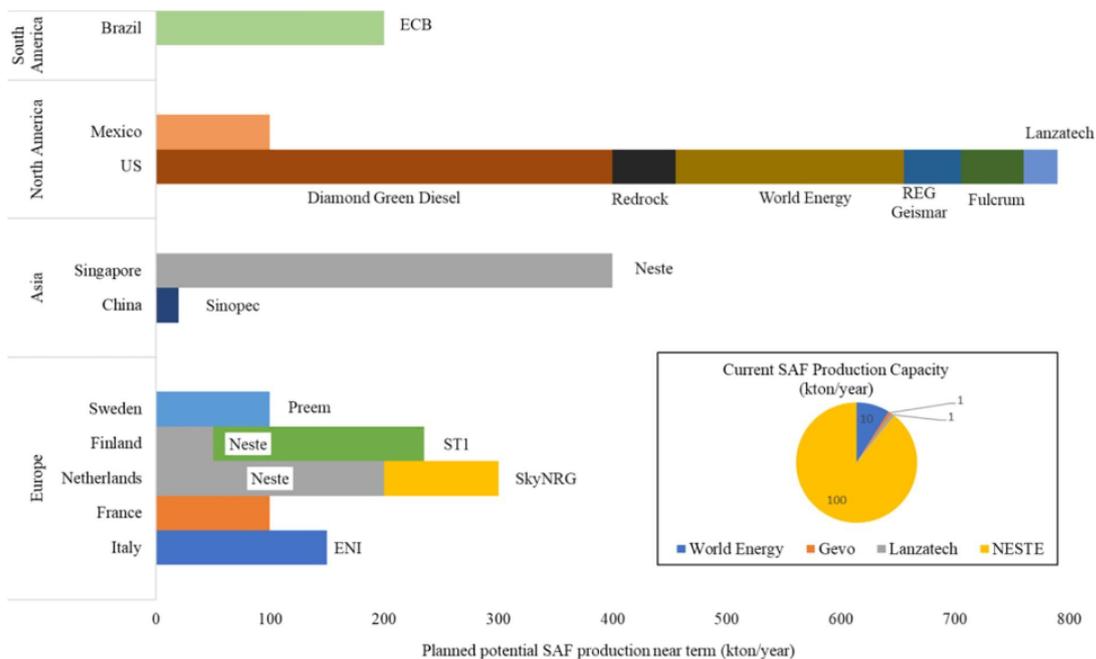
Sustainable aviation fuels must have functionally the same basic chemical makeup as fossil fuels. This is pivotal to ensure that manufacturers do not have to redesign engines or aircraft, and that fuel suppliers and airports do not have to build new fuel delivery systems, which could be necessary for alternatives such as hydrogen or electrification [6] [7]. The difference respect to conventional jet fuels is that they can be produced from non-petroleum-based renewable feedstocks. These include, municipal solid wastes, energy crops, agricultural and forestry residues, which

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allow offsetting the overall life-cycle greenhouses emissions, by the carbon dioxide absorbed by the biomass to grow.

In order to be eligible as a "Drop-in" fuels, SAFs must meet the strict guidelines regarding their physico-chemical characteristics such as viscosity, melting point, cloudiness, nonfreezing phenomena during low-temperature operations, and other properties to ensure optimum combustion performance under extreme conditions. In other words, they need to be certified with the standard ASTM D7566 (Specification for Aviation Turbine Fuels Containing Synthesized Hydrocarbons) requirements before they can be approved for any commercial activities [31].

The certification is strictly related to the conversion pathways from feedstock to jet fuel under analysis. As of July 2023, 11 conversion processes for SAF production have been approved, and 7 other conversion processes are currently under evaluation from ASTM International [25].

The following table summarizes the current approved conversion process for SAFs.

Table 2.2: Conversion processes approved by ASTM International [25]

ASTM reference	Conversion process	Abbreviation	Possible feedstocks	Maximum Blend Ratio
ASTM D7566 Annex 1	Fischer-Tropsch hydroprocessed synthesized paraffinic kerosene	FT	Coal, natural gas, biomass	50%
ASTM D7566 Annex 2	Synthesized paraffinic kerosene from hydroprocessed esters and fatty acids	HEFA	Bio-oils, animal fat, recycled oils	50%
ASTM D7566 Annex 3	Synthesized iso-paraffinic kerosene from hydroprocessed fermented sugars	SIP	Biomass used for sugar production	10%
ASTM D7566 Annex 4	Synthesized kerosene with aromatics derived by alkylation of light aromatics from non-petroleum sources	FT-SKA	Coal, natural gas, biomass	50%
ASTM D7566 Annex 5	Alcohol to jet synthesized paraffinic kerosene	ATJ-SPK	Biomass used for ethanol, isobutanol production	50%
ASTM D7566 Annex 6	Catalytic hydrothermolysis jet fuel	CHJ	Triglycerides such as soybean oil, jatropha oil, camelina oil, carinata oil	50%

ASTM D7566 Annex 7	Synthesized paraffinic kerosene from hydrocarbon - hydroprocessed esters and fatty acids	HE-HEFA-SPK	Algae	10%
ASTM D7566 Annex 8	Alcohol to jet derivative starting with the mixed alcohols	ATJ-SKA	Biomass used for ethanol, isobutanol production	100%
ASTM D1655 Annex A1	Co-hydroprocessing of esters and fatty acids in a conventional petroleum refinery	co-processed HEFA	Fats, oil and greases (FOG) co-processed with petroleum	5%
ASTM D1655 Annex A1	Co-hydroprocessing of Fischer-Tropsch hydrocarbons in a conventional petroleum refinery	co-processed FT	Fischer-Tropsch hydrocarbons coprocessed with petroleum	5%
ASTM D1655 Annex A1	Co-hydroprocessing of biomass	co-processed biomass	Biomass co-processed with petroleum	5%

As reported from the Table 2.2, bio-jet fuels are referred as a mixture of conventional aviation fuels and bio-based synthesized hydrocarbons rather than 100% bio-based compounds. Drop-in SAF needs to be blended with conventional jet fuel up to a maximum blend ranging between 5-50% depending on the process involved. It is done to ensure a balanced composition of paraffins, olefins, and aromatics, since, as already reported, the performance characteristics of bio-jet fuels in turbine engines are closely related to their chemical composition. In general, synthesized hydrocarbons have less complicated chemical composition than conventional jet fuels, which comprises hundred kinds of hydrocarbons. FT-SPK, HEFA and ATJ-SPK are made up by n-, iso- and cyclo-paraffins, and SIP mainly consists of iso-paraffins (a minimum of 97 %$_{wt}$ of farnesane). FT-SPK, HEFA, ATJ-SPK and SIP contains low amount of aromatics, while FT-SPK/A comprises up to 20 %$_{wt}$ of alkylated aromatics [34]. Aromatics play a critical role in traditional jet fuels for combustion characteristics and material compatibility. The absence of aromatics in the fuels causes the fuel to have a density below the minimum requirements and makes the elastomeric seal losing its proper swelling [35]. The seal shrinking can cause seal failures, thus damaging the system and promoting fire safety hazard, which is the reason why the lack of aromatics leads to a lower maximum permitted blending ratio.

Certain alcohol-to-jet (ATJ) pathways offer the potential to produce Sustainable Aviation Fuel (SAF) containing aromatics [12]. Specifically, the specification involves alcohol-to-jet synthetic paraffinic kerosene with aromatics (ATJ-SKA), developed by Swedish Biofuels technology [36]. This process utilizes single C2 to C5 alcohols or a combination of two or more C2 to C5 alcohols as feedstock. Unlike previously approved pathways, the Swedish Biofuels pathway is not restricted to a single feedstock and includes the production of aromatics. The fuel produced by Swedish Biofuels is indistinguishable from fossil kerosene in composition and properties, thanks to the flexible adjustment of aromatic content. Although ASTM D7566-23a currently allows the use of the jet fuel produced as a 50% blend with fossil kerosene, it marks a significant milestone in the sustainability journey and paves the way for 100% certification. Once ASTM publishes D7566-23a as a standard, it will become eligible for use in commercial airline fuel production, positioning ATJ fuels as a prospective option for achieving 100% SAF certification beyond current blending limits.

2.2 Conversion pathways

Several process technologies that convert biomass-based materials into jet fuel substitutes are currently available. Some of them operates on a commercial or pre-commercial scale, while others are still undergoing research and development [28]. These technologies are heavily reliant on the specific type of input feedstock since from them the pathway and the way of conversion (i.e., lipid, biological and thermochemical) vary. As presented in Table 2.2, the main conversion paths are briefly described as follows:

- **Fischer-Tropsch (FT):** Fischer-Tropsch synthesis is a process that produces hydrocarbons from syngas by using a metal catalyst. In the FT process, syngas, produced by gasification of carbon containing feedstock, enters a FT reactor where straight-chain alkanes are produced through a set of catalytic processes. FT fuels are typically free of sulfur and contain very few aromatics compared to conventional fossil-based fuel [36]. Currently, ASTM has certified two distinct FT processes. One yields a straight paraffinic jet fuel (SPK), while the other generates supplementary aromatic

compounds (SAK). The maximum blend ratio for both the options is set at 50%.

- **Hydroprocessed Esters and Fatty Acids (HEFA):** this method refines vegetable oils, waste oils, or fats into Sustainable Aviation Fuel (SAF) using hydrogen. In the initial step, the process eliminates oxygen through hydrodeoxygenation, subsequently, the straight paraffinic molecules undergo cracking and isomerization to attain the desired length for jet fuel [30]. The HEFA process shares similarities with the technique employed for producing Hydrotreated Renewable Diesel (HRD), although it involves more extensive cracking of longer-chain carbon molecules. The maximum blend ratio with conventional kerosene permitted by ASTM is 50%.

- **Synthesized Iso-Paraffins (SIP):** The SIP process commonly utilizes modified yeast to ferment sugar feedstock into a C_{15} hydrocarbon molecule called farnesene ($C_{15}H_{24}$), which must be further hydro-processed to form farnesane ($C_{15}H_{32}$), in order to be blended with conventional jet fuel [33]. Unlike the ATJ, which requires an alcohol intermediate, SIP directly produces alkane-type fuels from sugar. Feedstocks include starchy biomass such as sugar cane, beet, and maize, cellulosic biomass feedstocks (e.g., herbaceous biomass and corn stover), but even pretreated waste fat, oil, and greases also can be eligible feedstocks. Maximum approved blend ratio is 10%.

- **Alcohol-to-Jet (AtJ):** the pathway transforms alcohols into Sustainable Aviation Fuel (SAF) by eliminating oxygen and linking the molecules to achieve the desired carbon chain length through a process called "oligomerization". Then the olefins mixture is saturated with gaseous hydrogen and distillated to biojet fuel [37]. The alcohols are derived from cellulosic or starchy feedstock, via fermentation or gasification reactions. Ethanol and isobutanol produced from lignocellulosic biomass (e.g., agricultural residues) are considered favorable feedstocks, but other potential feedstocks (not yet ASTM approved) include isobutene, methanol, iso-propanol, and long-chain fatty alcohols [28]. In 2016 ASTM approved

the isobutanol process, and in 2018 the ethanol process with a 50% blend limit.

- **Catalytic hydrothermolysis (CH)** was developed to convert triglycerides to renewable fuels through a series of reactions, including cracking, hydrolysis, decarboxylation, isomerization, and cyclization, at temperatures ranging from 450 °C to 475 °C and pressures around 210 bars in the presence of water and a catalyst [28]. In this process, hydrogen from water is utilized for the hydrolysis of triglycerides and for hydrocarbon cracking. Thus, the use of hydrogen from non-renewable sources such as natural gas steam reforming is reduced, which lowers the carbon intensity of the resultant fuels. The final products include a mixture of n-alkanes, iso-alkanes, cyclo-alkanes, and aromatics, which can be fractionated into naphtha, jet fuel, and diesel fuel. Max blend ratio from ASTM spec. is 50%.

- **Hydroprocessed Hydrocarbons, Esters and Fatty Acids (HC-HEFA):** process, bio-derived hydrocarbons, as well as free fatty acids and fatty acid esters, are processed similarly to the HEFA process [38]. This involves hydroprocessing to saturate the hydrocarbon molecules and remove almost all oxygen. The choice between HEFA and HC-HEFA may depend on specific performance requirements, feedstock availability, and the desired characteristics of the biofuel. The Botryococcus braunii species of algae is a recognized source for this process, with a maximum blend ratio of 10%.

- **Co-processing:** Co-processing biomass feedstock with conventional fossil-based aviation fuel is an effective strategy to supplement fossil-based energy and reduce the capital cost associated with sustainable aviation fuel (SAF) production. There are two approved co-processing methods for SAF production: fats, oils, and greases (FOG) co-processing, and Fischer Tropsch (FT) co-processing [39]. It is important to note that co-processing is not a distinct SAF production pathway, but rather involves co-feeding renewable materials with crude oil-derived middle distillates in petroleum refineries [28]. As a result, co-processing methods are not listed in the D7566 specification but are included in the fossil jet fuel specification

(D1655) through an amendment. However, co-processed synthesized kerosene must adhere to both ASTM D1655 and D7566 specifications, ensuring additional quality control in the co-processing procedure.

Figure 2.2 presents a comprehensive summary of the main conversion pathways.

Figure 2.2: Several possible conversion pathways [25]
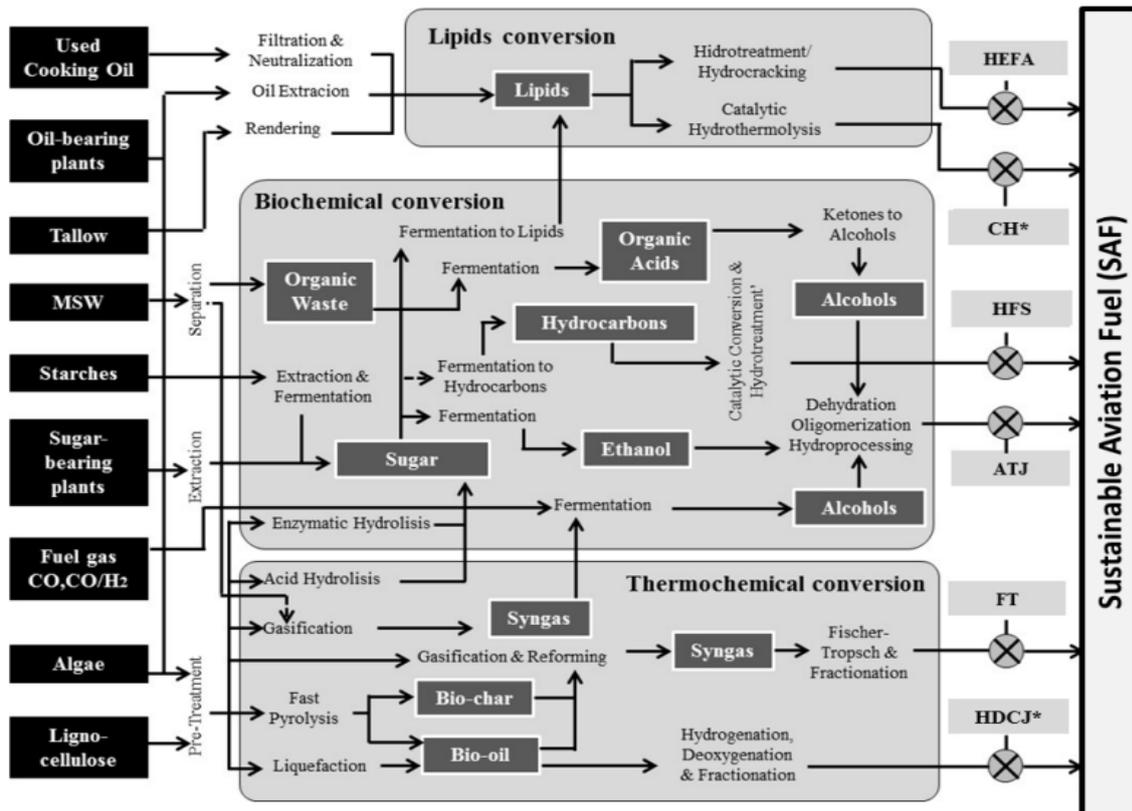
2.3 Biomass Feedstocks

2.3.1 First and second generation biomasses

First-generation and second-generation feedstocks are terms commonly used in the context of biofuels and renewable energy.

First-generation biofuels originate from biomass sources often utilized as food, such as corn, soy, palm oil, or sugarcane. These biofuels are derived through thermochemical or biochemical processes that convert the oils, sugars, and starches within the biomass into liquid fuels [40]. While first-generation biofuel markets and technologies are well established, they largely rely on crops that compete for arable land with those used for meeting human and animal nutritional needs [41]. Additionally, first-generation feedstock demands high quantities of water and fertilizer, as seen in corn cultivation, rendering it unsustainable.

Conversely, second-generation biofuels are derived from non-food biomass sources. This category encompasses fuels obtained from various agricultural residues and non-edible crops (such as agricultural and forestry waste, and herbaceous energy crops grown in abandoned land), along with municipal and general organic waste (such as biosolids, animal manure, paper waste, plastic waste, and post-consumption food). [42] The utilization of such energy crops and residues helps prevent conflicts between bioenergy production and the global food supply, enabling industrial countries to maintain their commitment to renewable energy plans and climate pledges.

The abundance and cost-effectiveness of lignocellulosic materials make them a desirable option for generating substantial quantities of fuel from renewable sources at a reasonable expense. Inexpensive by-products from the forestry sector and agricultural residues can serve as valuable raw materials [20] and rapid-growing energy crops like switchgrass, miscanthus, and reed canary can be viewed as potential long-term alternatives [21].

In the following paragraphs we will take a brief overview on the lignocellulosic feedstocks involved in the analysis.

2.3.2 Agricultural and Forestry residues

Agroforestry biomass refers to biomass that can be produced as a result of forestry and agriculture activities such as forestry management and agricultural waste management. In fact, forestry and agricultural waste can be considered an important energy source and as an alternative to traditional on-site disposal or burning leftovers [43]. In fact, improper waste disposal and long-term waste accumulation can lead to environmental problems, including foul smells, water pollution, eutrophication and increased biochemical oxygen demand. In addition, traditional waste reduction methods, such as burning, contribute to environmental issues by emitting pollutants like CO_2, CO, SO_X, NO_X, GHGs, ash, and unpleasant odors [44].

N. Scarlat et al. estimated the amount of agricultural residues potentially obtainable from wheat, barley, oat, rye, maize, rapeseed, rice, and sunflower, showing a potential of 212 million tonnes dry yr^{-1} (3715 PJ), for the period between 2000 and 2015 [20]. In 2020, a different study from Næss et al. assessed the spatial distribution of woody biomass potentials in 39 European countries [21]. The assessment considered stemwood, residues (branches and harvest losses), and stumps taking into account current and future developments in forest age-structure, growing stock, increment, and forest management regimes. Based on the study's findings, the total availability of forest biomass ranges from 357 to 551 million tonnes of dry matter annually.

Thus, residues may offer a significant opportunity for the production of bioenergy in various forms like electricity, heat, and liquid transportation fuels by using proper conversion technology to exploit their energetic value.

2.3.3 Perennial herbaceous energy crops

Grasslands, occupying a significant portion of Earth's land, play a crucial role in global agriculture, covering 20-40% of the planet and 38% of European agricultural land. These herbaceous areas are home of diverse perennial grass species classified under the Poaceae or Gramineae family [45]. Perennial grasses demonstrate high

efficiency in resource utilization, as the majority employ the C4 photosynthetic pathway, enhancing the capture of solar radiation and optimizing water utilization. They exhibit low nutrient requirements and can store nutrients in underground roots during winter. Furthermore, they show resistance and resilience to abiotic stresses, and their lignocellulosic cell wall structure provides natural resistance to pests and diseases [46]. Together with their contribution to ecosystem services, perennial grasses serve various purposes such as fodder, fiber, renewable energy production. On the other hand, the latest European directive on the promotion of renewable energies, suggested that some land categories should be excluded for such production such as highly biodiverse grassland, among others [47].

That is one reason why cultivating bioenergy crops on agriculturally degraded and abandoned lands is gaining importance as a sustainable approach to bioenergy production. This method offers environmental benefits and contributes to climate change mitigation without causing competition between food and fuel for land use or inducing direct and indirect land use change, with a consequential releasing carbon stored in forests. Lands categorized as agriculturally degraded or marginal lands have typically been left unused due to agricultural relocation or degradation from intensive use. Perennial grasses show high adaptability to marginal lands, in contrast to oil crops, sugars, cereals, and starch-rich crops used in biofuel production. Utilizing these lands for bioenergy production with low input, perennial grasses as feedstock appears promising, as it is likely to minimize negative impacts such as erosion and polluted runoff typical of conventional crops. [48]

Miscanthus (Miscanthus × giganteus), Reed canary grass (Phalaris arundinacea L.) and Switchgrass (Panicum virgatum L.) are considered the most suitable perennial grasses for the growth in European environmental conditions [49] and thus they have been chosen for our assessment.

- Miscanthus (Miscanthus × giganteus) is a C4 grass with a broad natural distribution, spanning tropical to subarctic regions. It thrives optimally at temperatures between 30 °C and 35 °C, maintaining productivity even in temperatures higher than 10 °C. However, yields decrease with increasing latitudes, and prolonged frost periods can lead to crop mortality. Typically,

miscanthus is harvested in late winter or early spring, exhibiting relatively high water-use efficiency compared to other C4 crops.

- Reed canary grass (Phalaris arundinacea), a C3 grass, grows in temperate climates across Eurasia and North America, flourishing in cool and moist conditions. It adapts to various water regimes and is resilient to disturbances like floods and droughts. Reed canary grass achieves peak photosynthetic rates between 20 °C and 25 °C, with optimal temperatures decreasing under increased water stress. Harvesting usually occurs in late winter or spring.

- Switchgrass (Panicum virgatum), a C4 grass native to North America, thrives in diverse environments, ranging from northern to southern regions. It exhibits optimal growth between 25 °C and 30 °C. Since severe drought events impacting yields, increasing water supply through irrigation during droughts can mitigate potential yield losses. Harvesting for switchgrass typically takes place during autumn. [50]

Through the identification of European abandoned cropland has been possible to estimate the amount of potential biomass productivity by using the perennial herbaceous crops which better adapt on the country specific climate condition. The results estimated current potential for dry biomass production in 28 selected European countries is approximately 98.4 million tons per year (ton db yr^{-1}). [51]

2.4 ATJ pathway

Producing sustainable aviation fuels from lignocellulosic biomass and residual wastes presents several challenges such as: 1) low energy density in feedstocks, 2) feedstock heterogeneity in chemical composition, physical properties, and moisture content, 3) the complex and capital-intensive nature of gasification, gas cleaning, and FT processes, and 4) low carbon efficiency in the overall production process [52]. The significance of alcohol production has grown due to its potential use as a drop-in transportation fuel. Nevertheless, Energy Information Agency (EIA) projections indicate a notable surplus of alcohols beyond what is necessary for gasoline blending [53]. With the ongoing shift toward electric road vehicles, this surplus creates opportunities for exploring alcohol-to-jet fuel pathways. The

process of converting alcohol to jet fuel involves several steps, but our initial focus is on examining the supply chain of selected alcoholic feedstocks for analysis, namely Ethanol, Isobutanol and hydrocarbon feedstock called Isobutene.

2.4.1 Chemical intermediates

Ethanol ($C_2H_6O_3$) is a simple, two-carbon alcohol typically made by fermenting sugar. Production of ethanol in this manner for human consumption in alcoholic beverages dates back thousands of years. Although the interest in alternative fuels for aviation is relatively recent, ethanol is not new to ground transport. Henry Ford used ethanol in a car in the 1880s, and is now frequently used as a fuel additive or blended with gasoline, such as E10 (10% ethanol, 90% gasoline) and E85 (85% ethanol, 15% gasoline) blends [54].

Bioethanol stands out as a promising alternative fuel for mitigating fossil fuel consumption in the transportation sector. Global bioethanol production reached 115 billion liters in 2019, with the USA and Brazil contributing 84% of the total output, followed by the European Union (5%), China (3%), Canada (2%), and India (2%) [55]. Primary feedstocks for bioethanol production in the USA, Brazil, and the EU involve various food crops: corn starch in the USA (constituting 94% of total production), sugarcane in Brazil (constituting 99% of total production), and sugar beet in the EU (constituting 40% of total production) [56].

Despite its popularity, ethanol has drawbacks such as being highly hygroscopic and corrosive, preventing its transport through existing fuel-supply pipelines. Additionally, its heating value is one-third lower than gasoline on a volumetric basis, although its lower stoichiometric air/fuel ratio and latent heat of vaporization partially compensate [57]. Due to these limitations, significant efforts have been made to develop a more attractive fuel for the transportation industry.

Isobutanol ($C_4H_{10}O$, sometimes represented as i-BuOH), is one of the four isomers of butanol and it stands out as a promising fuel for internal combustion engines due to its lower corrosiveness and hygroscopicity compared to ethanol. These qualities enable easy transport through existing fuel infrastructure [58]. Notably, isobutanol heating value is closer to gasoline, and it has a higher stoichiometric air/fuel ratio,

making it compatible with gasoline and with existing lambda control strategies, simplifying the adoption of i-BuOH as a drop-in oxygenate for the existing vehicle fleet [59]. Beyond serving traditional markets like solvents and coatings, isobutanol can be chemically converted into isobutylene, a versatile building block for various petrochemical products. Gevo's GIFT Process, combining synthetic biology and industrial chemistry, offers a scalable method for i-BuOH production, contributing to the development of an innovative pathway to produce sustainable aviation fuel. Since 2014, the Gevo plant in Luverne, MN, has been concurrently operating the production of isobutanol alongside ethanol in a side-by-side operation, as shown in Figure 2.3 [60].

Figure 2.3: Schematic representation of the i-BuOH-Ethanol side-by-side dry-mill process [60]
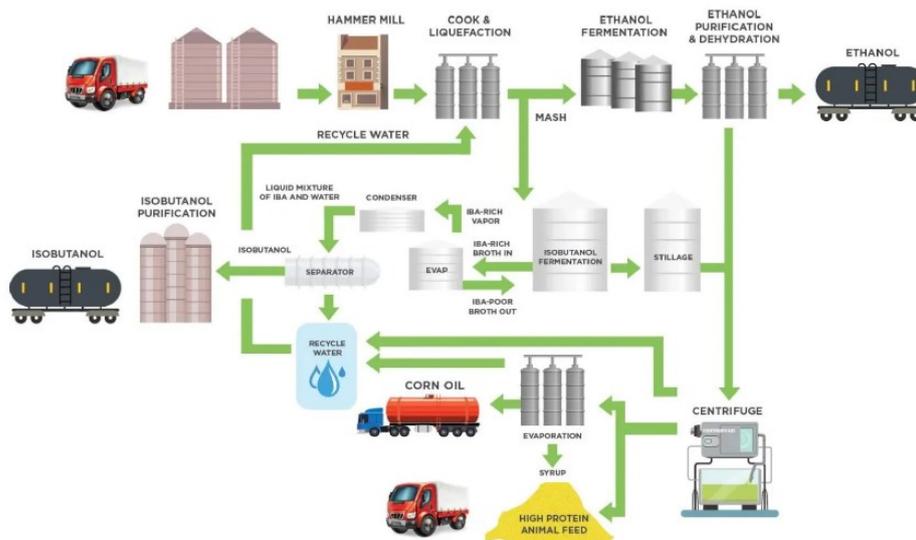
Isobutene, or isobutylene (C_4H_8), is a hydrocarbon gas, originally obtained from oil refinery streams, which holds a significant role among the four isomers of butene due to its heightened reactivity in addition and polymerization reactions, making it a key player in the chemical industry. Currently, butenes are primarily derived as co-products from crude oil refining cracking processes. However, considering its global production, projected market growth, and diverse applications, there exists substantial potential to replace fossil isobutene with a bio-based equivalent, contributing to the decarbonization of the chemical industry. [61] Even though it is not an alcohol, high interest has been given for its application in sustainable aviation

fuel (SAF) production by means of the ATJ pathway, because of a novel process developed by Global Bioenergies (GB) closely mirrors Gevo's pathway from isobutanol to jet fuel, being isobutene a chemical intermediate of such route. GB's process involves microorganisms directly producing isobutene during fermentation, followed by a series of upgrading steps including oligomerization, hydrogenation, and fractionation [26].

In the table 2.2 the physico-chemical characteristics of those fuel are compared.

Table 2.2: Physico-chemical properties of Ethanol, Isobutanol and Isobutene [62] [63]

Properties	Ethanol	Isobutanol	Isobutene
Formula	$C_2H_6O_3$	$C_4H_{10}O$	C_4H_8
Molecular mass [u]	46.1	74.1	56.1
Carbon content [%]	52	65	85.7
Density [kg/m³]	789	802	626
Energy density [MJ/l]	21.4	26.6	28.2
LHV [MJ/kg]	26.7	33.3	45.1
Heat of evaporation [MJ/kg]	0.92	0.69	0.39
Boiling point [°C]	78	107.9	-6.9
Explosive limit concentration [%vol]	3.3-19	1.7-11.9	1.8-9.6
Flash point [°C]	13	28	-76.1
Autoignition temperature [°C]	363	415	465

2.4.2 Biological fermentation to produce chemical intermediates

In recent decades, there has been a notable interest in using biological fermentation techniques for producing various biofuels, such as bioethanol, biobutanol, biobutene, biodiesel, vegetable oils, bio-based methanol, and biohydrogen. This focus is driven by the potential to utilize abundant biomass, particularly lignocellulose, in contrast to traditional chemical synthesis methods reliant on fossil resources. [64] The process of converting biomass into alcoholic or chemical intermediates shares common steps across all analyzed biofuels, with variations in fermentation and recovery processes specific to each type.

1. **Pretreatment**

The initial phase in the production of alcohol from lignocellulosic biomass involves pretreatment, a process aimed at breaking down the complex lignocellulose structure to enhance the accessibility of cellulose and hemicellulose for enzymatic

hydrolysis. This step, also known as pre-hydrolysis, disrupts the cell wall structure, releasing lignin and soluble sugars (glucose, arabinose, xylose, galactose, and mannose). Pre-hydrolysis of cellulose and hemicellulose improves the enzymatic digestibility of the feedstock [65]. Grasses, with their low lignin content, benefit from milder pretreatment conditions, while softwoods pose challenges due to their structural complexity and high lignin content [66]. Various techniques, including physical, chemical, and biological methods, have been explored for pretreatment. This stage is considered the most challenging in the biorefinery process, accounting for over 40% of the total processing cost. Without pretreatment, saccharification of lignocellulosic materials may yield total sugar below 20%, whereas pretreatment methods can achieve total sugar yields ranging from 60% to 90% [67].

2. Enzymatic Hydrolysis

The objective of biomass saccharification and hydrolysis is to break down the intricate structure of biomass into fermentable sugars and/or other monomeric components. Historically, two fundamental methods for biomass saccharification have been acid hydrolysis and enzymatic hydrolysis. Acid hydrolysis, an established and cost-effective technique, induces structural changes in biomass, enhancing accessibility for biofuels conversion. On the other hand, enzymatic hydrolysis is regarded as a promising method due to its lower energy consumption and mild environmental conditions [68].

3. Fermentation

The fermentation processes for ethanol, isobutanol, and isobutene share a common foundation in converting sugars to alcohols through microbial activity, but they diverge in crucial aspects. Ethanol production relies mainly on the yeast Saccharomyces cerevisiae, while isobutanol and isobutene fermentation may involve bacteria like Clostridium species or engineered strains of bacteria like Escherichia coli, as native bacteria and yeasts yield insufficient amounts [62] [69]. Simultaneous saccharification and fermentation (SSF), combining hydrolysis and fermentation in a single step, is preferred by many industries due to lower costs, fewer inhibitory compounds, and a lower risk of contamination. However,

optimizing the pH is a concern since conditions may vary for hydrolysis and fermentation, necessitating an equilibrium for efficient operation [70].

4. Product Recovery

The post-fermentation recovery process includes distillation, where the fermentation broth is heated to separate the biofuel from water based on boiling points and additional purification steps [71] [72] [73].

Common by-products of these procedures are lignin residues and wastewater. Lignin can be combusted in a CHP plant to generate electricity and heat, reducing external inputs for the overall process. Wastewater can be treated for recirculation in the system or to produce valuable co-products like biogas. However, specific conditions and methods may vary depending on the microorganism and fermentation pathway, such as gas stripping, adsorption, or solvent extraction. Due to the extensive literature and diverse processes, the thesis will not enter into details, but refer on the selected processes outlined in the method chapter.

2.4.3 Jet fuel production from chemical intermediates

To produce drop-in alternative jet fuel from alcohols, it is essential to minimize the differences in physical and chemical properties between chemical intermediates and conventional jet fuel. The process of production hydrocarbons in the jet fuel range from the alcohols generally undergoes a four-step upgrading process. First the alcohol dehydration generates olefins, then the olefins are oligomerized in the presence of catalysts to produce a middle distillate. Next, the middle distillates are hydrogenated to produce the jet-fuel-ranged hydrocarbons and final step is the distillation.

Figure 2.4: Isobutanol ATJ-SAF [82]
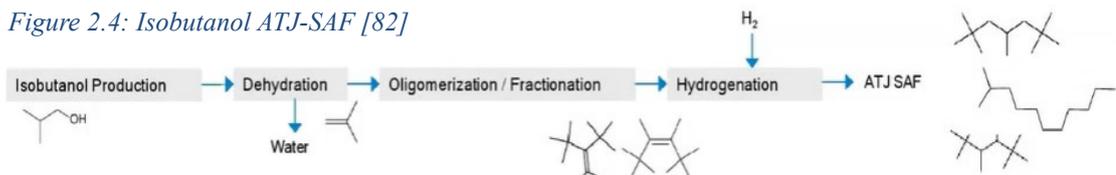
Figure 2.5: Ethanol ATJ-SAF [82]
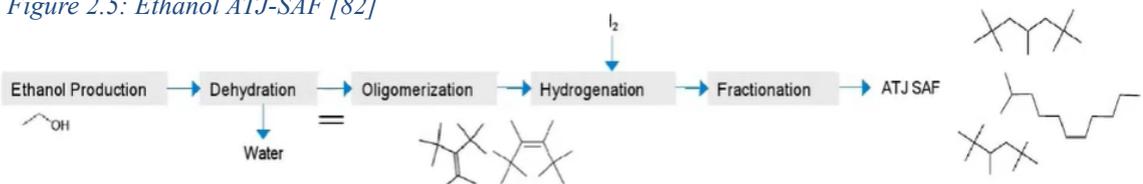
In the ethanol dehydration process, common catalysts such as Al_2O_3, transition metal oxides, zeolite catalysts, and heteropoly acid catalysts are utilized [74]. The resulting ethylenes then undergo catalytic oligomerization, with the catalysts being either homogeneous or heterogeneous. Steven et al. [75] detailed an ethylene oligomerization process using cationic (α-Diimine) nickel(II) catalysts treated with aluminum alkyl activators, achieving a selectivity of up to 96% for linear olefins under optimized conditions.

Even though ethylene is one of the most usable light olefins to oligomerize and polymerize, its suitability is significantly reduced due to its tendency to form C_2-C_8 oligomers instead of C_{10+}. [76] In industrial oligomerization processes, a broader distribution of carbon numbers is generated, including 5% C_4; 50% C_6–C_{10}; 30% C_{12} and C_{14}; 12% C_{16} and C_{18}; and 3% C_{20} and C_{20+} [69], operating at 200 °C and 250 bar. The resulting olefins are distilled into diesel and jet-range fuels, along with light olefins (C_4–C_8) [28]. Distilled light olefins are recycled back to the oligomerization step, as depicted in Figure 5. Products in the jet fuel range (C_9–C_{16}) can undergo hydrogenation at temperatures of 370 °C, using hydrogen feed at 5% by weight over a palladium or platinum on activated carbon catalyst [73]. The alkanes (C_9–C_{16}) produced from the hydrogenation step are suitable for renewable jet fuels.

Isobutanol, derived from processes like Escherichia coli fermentation, undergoes dehydration to produce a mixture of isobutene, n-butene (1-butene), and 2-butene (cis-2-butene and trans-2-butene). Acidic catalysts, such as ZSM-5 zeolites, Y-type zeolites, and Amberlyst acidic resins, catalyze the dehydration reaction, influencing the selectivity of isobutene and overall linear butenes. The reported isobutanol dehydration yield is 99.1%, with a selectivity of 95.1% isobutene, 1.6% 1-butene, 0.5% trans-2-butene, and 1.9% cis-2-butene at 325 °C using ZSM-5 catalyst [73]. Isobutanol can also be converted into isobutene with a 98% conversion at 310 °C over a γ-Alumina catalyst. Isobutene can further be converted to oligomers, trimers, and tetramers at 100 °C using an Amberlyst-35 catalyst, resulting in 20%, 70%, and 10% for C_8, C_{12}, and C_{16} olefins, respectively. 1-butene is converted into 25%, 24%, 17%, and 25% to C_8, C_{12}, C_{16}, and C_{20} olefins, respectively, yielding an overall 1-butene yield of 96% with 4% unreacted.

To enhance jet and diesel yields, C_8 olefins can be distilled and sent for additional dimerization at 116°C over a Nafion catalyst, as shown from Figure 4. Alternatively, C_8 olefins can be converted into $C_{16}H_{32}$ through dimerization or reacted with butenes to produce C_{12} olefins, contributing to an increase in C_{12} and C_{16} for jet-range chemicals.

The final stage consists of saturating olefins mixture from the oligomerization with gaseous hydrogen. It converts the trimers and dimers into iso-paraffines since its olefinic character, and foreseeable low oxidation stability would hinder their direct use as a biojet fuel blending component. Through the distillation process, we can effectively isolate bio-jet fuel from the rest of the hydrocarbons.

The Isobutene route mirrors the I-BuOH process, with the exception that the dehydration process is excluded being isobutene the most common dehydrated form of isobutene. Isobutene SAF is fully iso-paraffinic and rich in C_{12} and C_{16}, that is why it is currently seeking ASTM approval by inclusion in D7566 Annex 5, given the very close similarity with i-BuOH ATJ SAF. [77]

The processes just described are represented by the flowchart depicted in Figure 2.6.

Figure 2.6: Pathways to obtain bio-jet fuel from different alcohol sources [67]
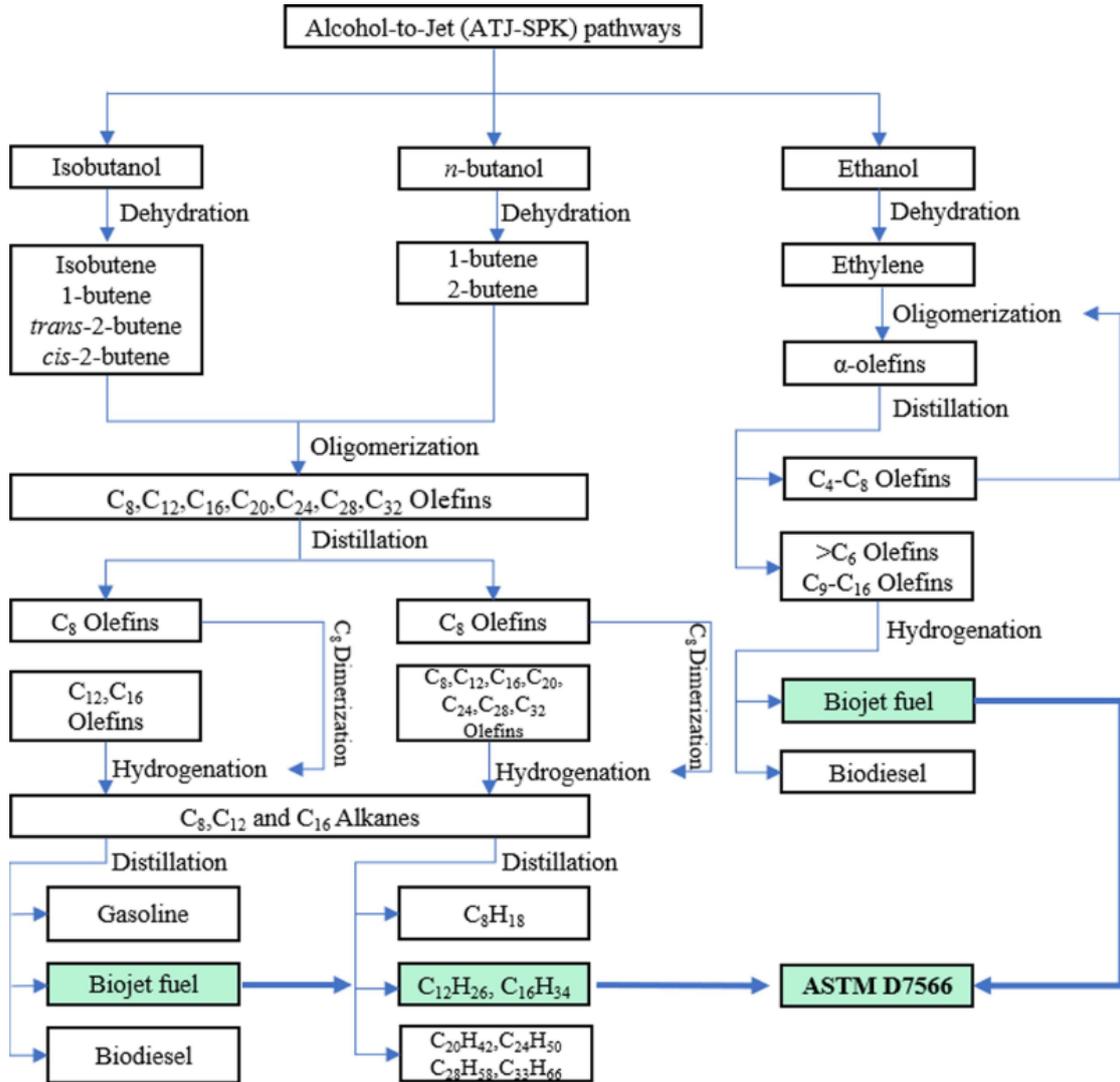
Methods

The methodology employed in a study plays a pivotal role in comprehending the structural framework of the research. It delineates the approach to data collection, as well as the tools and materials utilized. The methodological choices significantly contribute to the overall reliability and validity of the study.

In this chapter, we explore the methodologies employed to define diverse supply chains and compile a comprehensive life cycle inventory for the life cycle assessment. The well-to-wings processes are constructed by linking various studies pertaining to each phase of the alcohol to SAF supply chains. The studies were specifically selected from a broader spectrum of researches, prioritizing reliability, comprehensive descriptions of the processes, reported data accuracy, and thorough results discussion. The reasoning behind each selection will be clarified in the following paragraphs.

3.1 Identification and description of supply chains

This thesis identifies three primary routes that culminate in the production of sustainable aviation fuels, each involving distinct chemical intermediates: Ethanol, Isobutanol, and Isobutene. The well-to-wings analysis encompasses several steps outlined in the figure, including biomass collection, transportation of feedstock to the biorefinery plant, conversion stage and transportation from the biorefinery to the airport farm, as represented in Figure 6.

It is important to highlight that the carbon dioxide (CO_2) emissions directly associated with the biorefinery conversion stage and the combustion of SAF are classified as biogenic CO_2. This means that the emitted CO_2 originates from biomass, having been absorbed from the atmosphere during its growth, does not contribute to the overall increase in greenhouse gas emissions in the atmosphere. Also the Intergovernmental Panel on Climate Change (IPCC) global warming methodology does not take biogenic CO_2 into account when assessing the impact on climate change. Therefore, emissions from biogenic sources are not considered in calculations of Global Warming Potential (GWP) estimates. Consequently, the GHG emissions attributed to direct biorefinery plant emissions in the evaluated

processes are exclusively derived from associated underlying activities, such as inputs/outputs supporting process operations within the facility.

Figure 3.1: Conversion route from feedstock farming to SAF combustion

Farming and collection — Transportation to biorefinery — Conversion to SAF — Transportation to airport — SAF combustion

3.1.1 Biomass farming, collection and transportation to biorefinery plant

Concerning biomass collection, we rely on findings from two distinct studies. N. Scarlat et al. [20] evaluate the potential of sustainable crop residues in European Union Member States. Such study allows to compute the country-specific emissions associated with biomass transportation to the biorefinery plant by considering the spatial distribution of biorefinery plants in each country and assessing the average distance of such facilities. The emissions linked to residue production, attributable to diesel, lubricant oil, fertilizers, and pesticides, are not included in this analysis, since they have been entirely allocated to the primary product of the crop (e.g., wheat, rye, barley, oats, maize, rice, rapeseed, and sunflower), whereas, the data related to biomass collection were excluded, as they were found to have a negligible impact on the overall emissions. Watanabe et al. [51] provided the data relative to herbaceous energy crops cultivated on marginal lands in 28 European countries. To identify the abandoned cropland, it was used the land cover data from European Space Agency Climate Change Initiative (ESA-CCI) by combining several earth observation products and by using the GlobCover unsupervised classification chain. The total biomass production from the selected bioenergy crops is based on the yields of perennial grasses under rainfed water supply according to the model Global Agro-Ecological Zones (GAEZ), as outlined in a previous study conducted by Fischer et al. [78]. The current potential of dry biomass production in the selected 28 European countries is estimated to be approximately 98.4 $Mton_{db}$ per year. The country-specific environmental burdens for miscanthus, reed canary grass, and switchgrass include the major farming activities (soil preparation, fertilization,

harvesting) and transport to the biorefinery plant and are based on the life cycle inventories from Gvein et al. [79].

3.1.2 Conversion to SAF by ATJ pathways

The production of alcohol and chemical substances occurs in biorefineries where the lignocellulosic biomass coming from the fields is first chipped in smaller particles and then processed in the biorefinery through the step described in the previous chapter: Pre-treatment, Saccharification, Fermentation, Product recovery. Then, we assumed the biorefinery boundary comprises also the conversion plant to produce bio jet fuel from chemical intermediates, this is the so called "standalone" approach [80]. Each conversion plant taken in account, from which data were collected, is based on different Life Cycle Assessments (LCA) or Techno-Economic Analysis (TEA) from literature, based on either real biorefineries or simulated through Aspen Plus.

<u>Chipping and storage</u>

The chipping and storage stage remains the same across all three conversion routes. Figure 3.2 illustrates a simplified process flow diagram. The plant receives dump trucks loaded with lignocellulosic biomass at a rate to meet production demand. Unloading these trucks using the dumper takes approximately ~10 minutes. The dumpers discharge into hoppers, which direct the biomass to a series of conveyors leading to a covered storage section. Utilizing two storage domes allows for continuous operation, as one dome can be loaded while the other is emptied for the conversion process. Wheel loaders handle the distribution of biomass within the storage domes and load conveyor belts to transport the biomass to the chippers. In this segment, two different chippers are employed: chipper 1 reduces the size to a 400 mm chip length, and chipper 2 mills the chips to a 40 mm chip length. A disc scalping screen is employed to screen large and oversize biomass chips, which are then returned to chipper 2. Finally, the biomass is stored in a chip silo equipped with a discharger to regulate the biomass flow delivered to the pretreatment process.

The storage and chipping area is analyzed separately with the data referring to a process simulation conducted by Morales et al. [65].

Figure 3.2: Description of the storage and chipping stage [65]
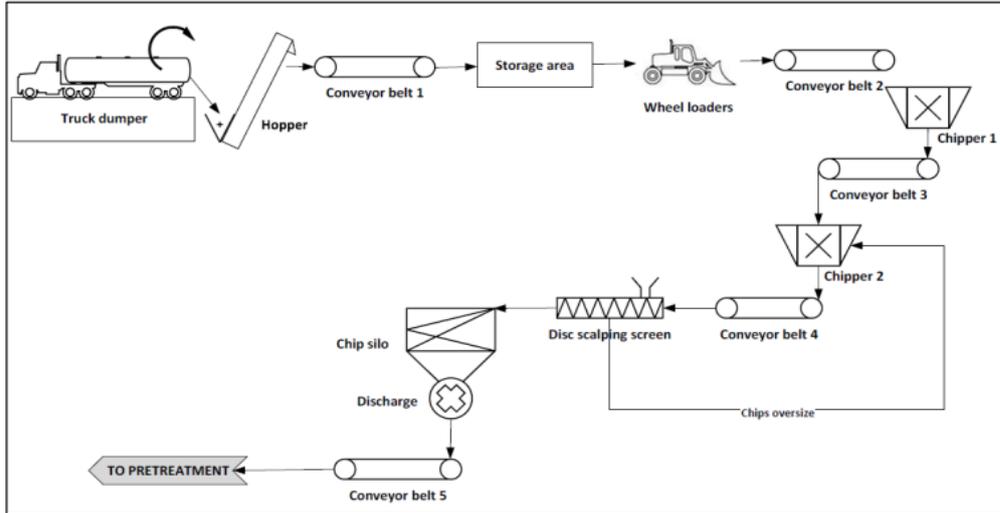
Isobutanol Route

Tao and al. [62] developed the well-to-wings analysis for lignocellulosic isobutanol derived from corn stover. The process design includes feedstock handling and storage, product purification, wastewater treatment, lignin combustion, product storage, and all other required utilities. Acid pre-treatment is employed, with the addition of ion exchange columns to the process to eliminate inhibitors such as acetates, salts, and various organic acids. The pre-treated hydrolysate undergoes conditioning with ammonia to achieve the appropriate pH for enzymatic hydrolysis. Subsequently, enzymatic hydrolysis of the remaining cellulose and hemicelluloses takes place, initially through partial hydrolysis. The resulting slurry is then batched to a system of parallel anaerobic bioreactors, where hydrolysis is completed. The slurry is then cooled to 32 °C and inoculated with organisms for fermentation. The anaerobic process for isobutanol production utilizes improved E. coli strains. Continuous vacuum stripping is applied during butanol fermentation, as illustrated in the accompanying Figure 7. The vacuum stripper condenser and the recycling fermentation stream maintain the fermenter broth at no more than 2%wt of i-BuOH condensate. The sugar-to-isobutanol conversion yield is estimated at 85%, with the remaining sugar converted to cell mass and other by-products. The resulting fermentation broth, referred to as "beer", is directed to the product recovery stage.

Plant wastewater streams undergo treatment through anaerobic and aerobic digestion to produce methane-rich gas (biogas) and sludge. The treated water is suitable for recycling and is reintroduced into the process. Solids and sludge from the fermentation process, along with biogas from anaerobic digestion, are combusted in a fluidized bed combustor to generate high-pressure steam for electricity production and process heat. The pre-treatment reactor and distillation areas account for the majority of the process steam demand. Excess steam produced in the boiler is converted to electricity for in-plant use and can be sold to the grid as a co-product.

Figure 3.3: I-BuOH fermentation with simultaneous stripping and purification process block flow diagram [62]
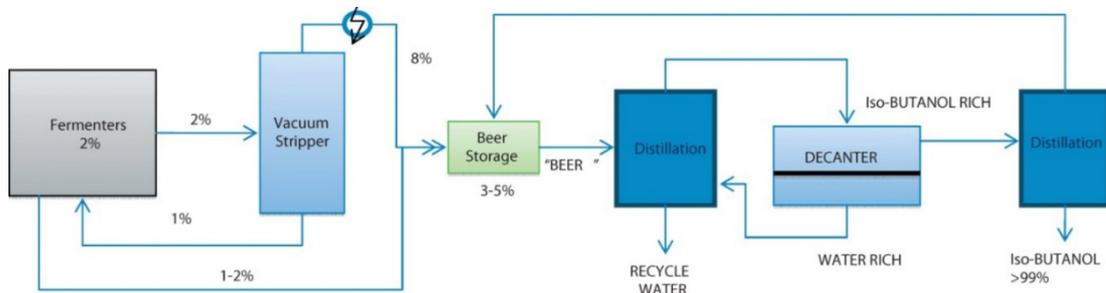
The study in question has been deemed the most reliable for isobutanol production, primarily due to its detailed description of the production design and its substantial number of citations, totaling 169. Notably, the inclusion of yeast in the inventory is absent, and while the study itself does not offer a specific rationale for this exclusion, it aligns with a consistent pattern observed in the literature. In fact, other studies similarly overlook the contribution of yeast in i-BuOH production, a practice that may be justified by the relatively minimal impact of yeast input, due to small amount [17]. Figure 8 depicts the main steps and input/output flows of isobutanol production plant considered in this thesis.

Figure 3.4: Flowchart of lignocellulosic i-BuOH production plant
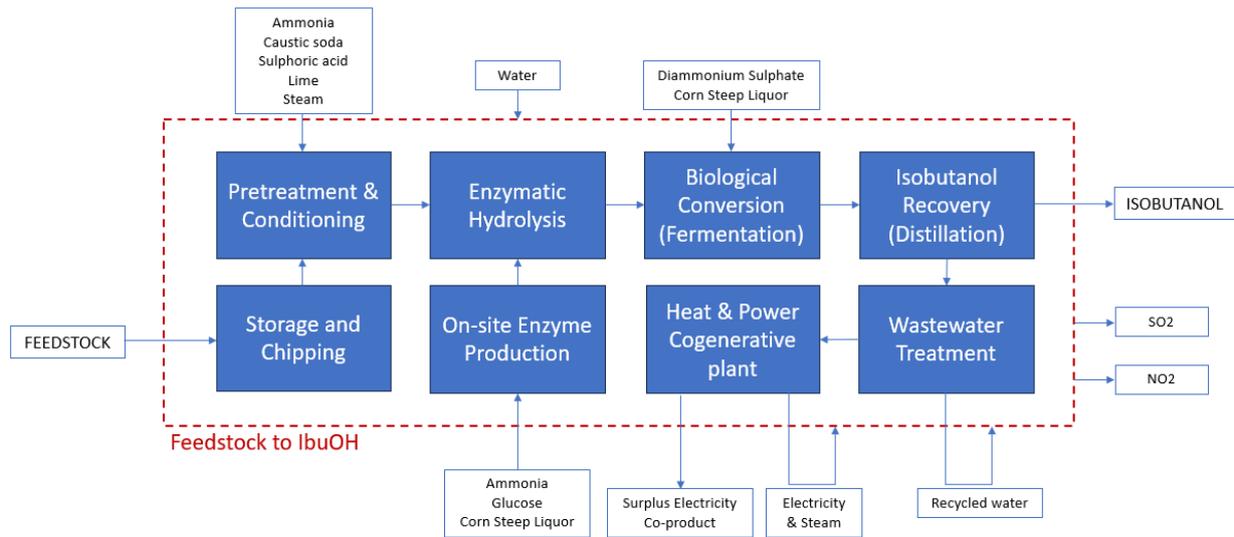
Isobutanol produced by fermentation, undergoes a process involving dehydration, oligomerization, and hydrotreatment, represented in Figure 9, that closely resembling the Gevo method. In fact, the Massachusetts Institute of Technology (MIT), on behalf of ICAO, utilized process data provided by Gevo under a nondisclosure agreement. These data were employed to estimate jet fuel yields from i-BuOH and determine the necessary requirements for heat and hydrogen in the upgrading process. The distillation process yielded the following proportions of hydrocarbons, as reported in the analysis: 37,2%wt (Diesel), 2,4%wt (Heavy oil), 90,4%wt (Jet fuel) [17].

Figure 3.5: Flowchart of i-BuOH conversion to jet fuel & co-products
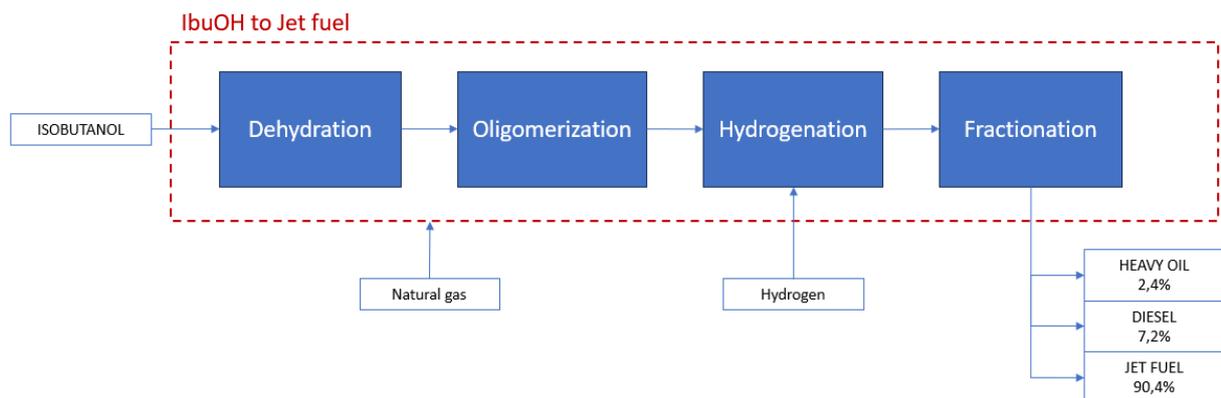
Ethanol Route

Concerning the ethanol pathway, this study explores ethanol production from agricultural residues, with a specific focus on the corn stover ethanol production process outlined in the CORSIA Supporting method [14]. Drawing from a

comprehensive review of literature spanning from 2000 to the 2022, with an emphasis on U.S.-related studies, a synthesis of data was conducted. The CORSIA supporting method reviewed and collected the life-cycle inventory of the ethanol-to-jet process from various research papers as well as the industry data, in collaboration with Argonne National Laboratory (ANL) and National renewable energy laboratory (NREL). The concentration on these organizations stems from their provision of detailed models and data across various parameters within the corn stover pathway, filling gaps in alternative data sources. Given the extensive range of literature from which the data are derived, specific process details are not extensively disclosed, as they may vary according to the specific conversion process. Nevertheless, the provided ethanol life cycle inventory (LCI) data are deemed more reliable and representative of the average lignocellulosic ethanol supply chain. The bioethanol production facility considered for the analysis encompasses seven primary sections: Storage and chipping, Pretreatment, Enzymatic hydrolysis, Fermentation, Bioethanol recovery, Cogeneration of heat and power, and Wastewater treatment. Cogeneration involves the production of heat and electricity by burning combustible solids and biogas from various process streams, including distillation solids, biogas, sugars from water treatment, and saccharification lignin. The summarized process steps are presented in Figure 3.6.

Figure 3.6: Flowchart of lignocellulosic bioethanol production plant
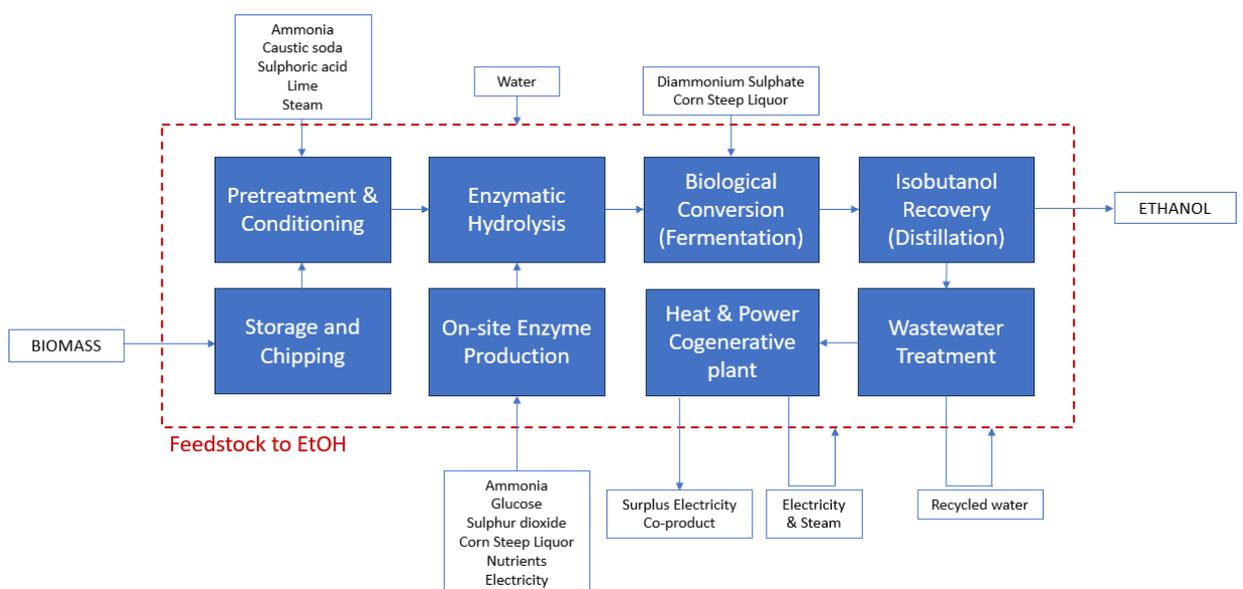
The second-generation ethanol produced from agricultural residues is subsequently converted to drop-in fuel via dehydration, oligomerization and hydrotreating.

Figure 3.7 outlines the parametric assumptions for ethanol-to-jet (ETJ) production processes, which are based on the TEA conducted by Wang et al. [77]. The analysis focused on data for the standalone configuration, which operates under the assumption that the ATJ facility acquires ethanol either from the market or through a separate ethanol production process.

The process begins by catalytically removing oxygen from ethanol molecules through dehydration, yielding ethylene. Subsequently, ethylene undergoes catalytic oligomerization, forming linear or branched α-olefins with a hydrocarbon distribution ranging from C4 to C32. As jet fuel has restrictions on olefin content, the final step involves hydrogenating the α-olefins to produce paraffins.

As documented in the analysis, the distillation process resulted in the following hydrocarbon proportions: 8.96%wt for Diesel, 16.1%wt for Gasoline, and 75.1%wt for Jet fuel [80].

Figure 3.7: Flowchart of ethanol conversion to jet fuel & co-products
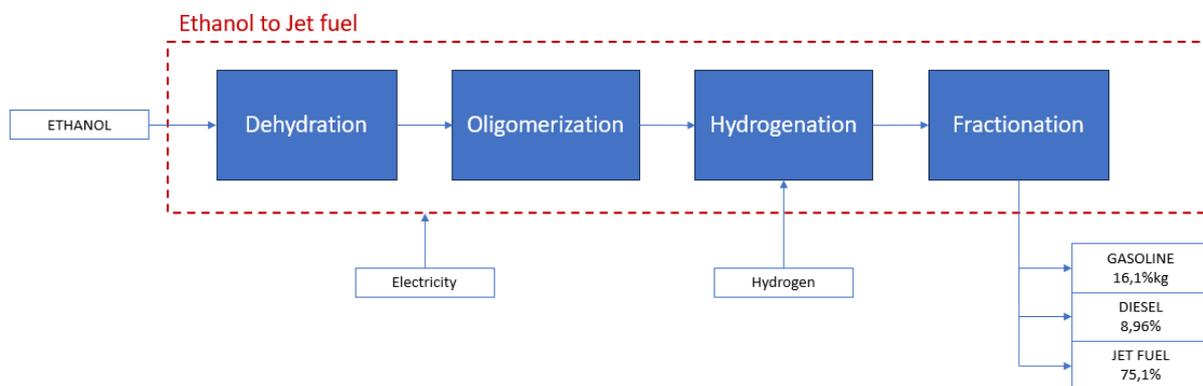
Isobutane Route

To identify the lignocellulosic isobutane supply chain and enable its conversion into Sustainable Aviation Fuel (SAF), we referred to a research paper authored by S. Puschnigg et al., 2023 [81]. The paper outlines the development of a biorefinery designed for the transformation of softwood residues into sustainable aviation fuel, by combining the knowledge and technologies of several technology providers during the REWOFUEL 2022 project [82]. This project aimed to demonstrate the performance, reliability, environmental impact, and socio-economic sustainability

of the entire value chain. The key processes involved the conversion of residual softwood into hydrolysate (RWH), the fermentation of RWH into bio-Isobutene (bio-IBN), and the subsequent conversion into biofuels.

The research explored eight different scenarios related to the supply of process energy and the utilization of by-products. Thermal energy can be sourced from either a natural gas or a lignin boiler, with electricity obtained from the public grid in this configuration. When integrating a Combined Heat and Power (CHP) plant (powered by either natural gas or lignin), it not only provides thermal energy but also generates electricity and any deficit in electricity is supplemented from the public grid. None of the scenarios in this study involve an electricity surplus available for sale, though future technological advancements and efficiency improvements may change this.

The scenarios considered in this thesis were the Lignin-Cogeneration Heat and Power (LI-CHP) scenarios, which involve the integration of a Combined Heat and Power (CHP) plant fueled by the by-product lignin obtained from sugar separation. This integrated system not only generates thermal energy but also produces electricity, thereby mitigating the need for external energy sources. Only the lack of electricity is consumed via the public grid.

The by-products generated in the value chain include lignin, ethanol, sludge, and microbial biomass. These by-products can find applications across various industries. Opting for on-site utilization of lignin for thermal and electricity production reduces the amount of lignin available externally (e.g., in the asphalt industry as a bitumen substitute). However, this on-site usage of lignin decreases dependence on external energy suppliers, while other by-products like ethanol, fertilizer, and animal feed remain unaffected.

Sustainable Aviation Fuel (SAF) undergoes production in multiple process units, including wood-to-sugars, fermentation, purification, and conversion. Figure 3.8 illustrates a comprehensive description of the system boundary, the steps involved in the SAF supply chain, and the possible scenarios developed in the mentioned study. The initial phase involves transporting sawdust to the biorefinery via trucks. In the wood-to-sugars unit, sugars (C6 and C5) present in the cellulose and hemicellulose of sawdust undergo pretreatment and enzymatic hydrolysis, resulting

in residual wood hydrolysate. The separated C5 sugars are then converted into bio-ethanol, while lignin, another by-product, can be utilized on-site for energy production or as a material substitute. Lignin finds applications as a bitumen substitute in the asphalt industry and in end-use applications like phenol-formaldehyde resins and bioplastics filler.

The residual wood hydrolysate (C6 sugars) is fermented to produce bio-isobutene, employing modified bacterial Escherichia coli (E.coli) strains. This method, previously detailed by Fazeni-Fraisl and Lindorfer (2022) [69] and Lopes et al. (2019) [61] for various lignocellulosic feedstocks, is an innovative process currently under development to enhance performance and yield. The by-products of fermentation include sludge and microbial biomass, serving as potential fertilizer and animal feed, respectively. The microbial biomass, consisting of amino acids, can be used as protein feed, particularly in broiler and piglet feed, though it requires approval from the European Food Safety Authority due to containing inactivated genetically modified organisms.

After fermentation, bio-isobutene is purified using an adsorption/desorption column principle. In the final step, bio-isobutene undergoes oligomerization and hydrogenation to form SAF isoparaffins.

The "off-site (auxiliaries)" section, an integral component of the biorefinery, encompasses storage and logistics elements such as conveyor belts for raw material transport, pumps for various fluids, storages, agitators, blowers, and heat exchangers, all essential for the overall operation.

The production of bio-isobutene from residual wood hydrolysate is an innovative process and currently in development to further increase the process performance and yield and Global Bioenergies, a prominent leader in this field, has obtained several patents for its research in this field. As a precaution to preserve technological leadership, the company refrains from providing detailed information regarding the conversion process.
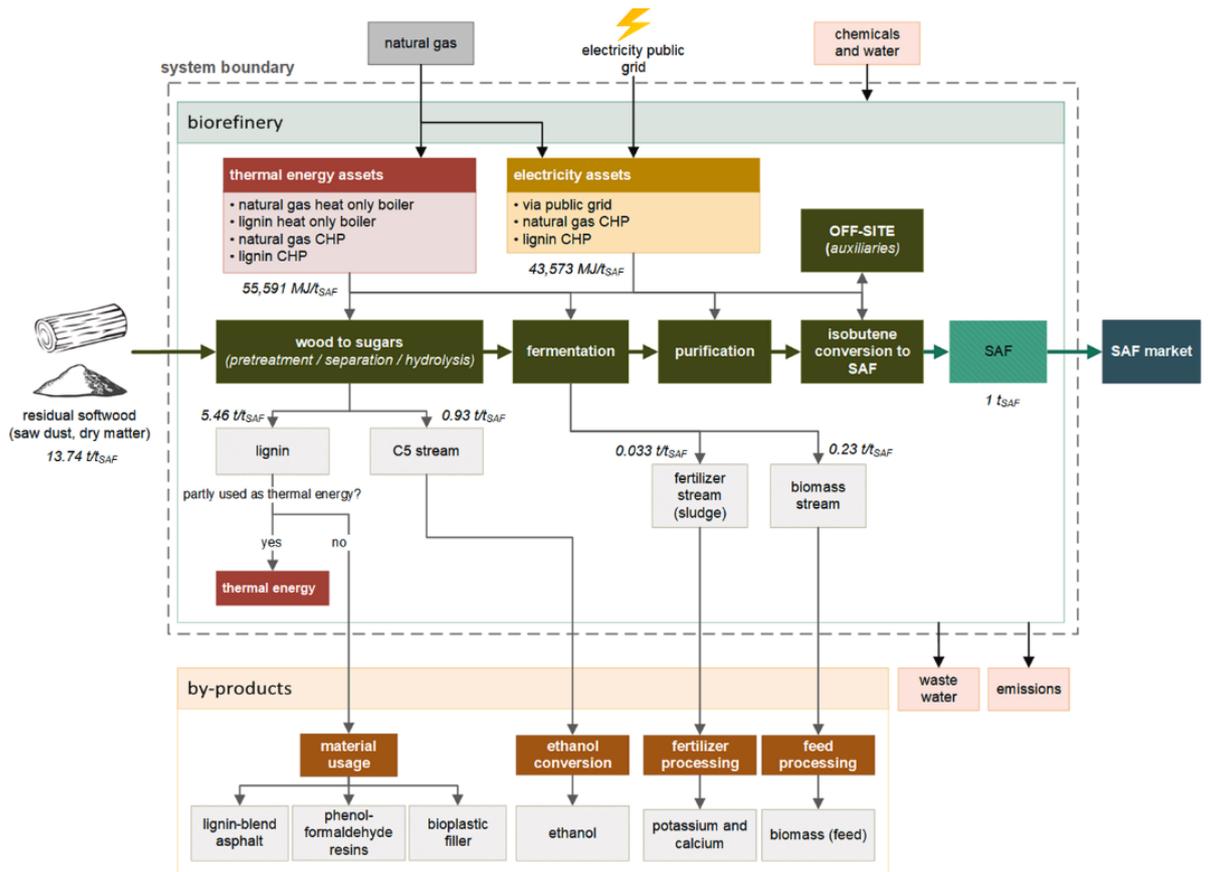
Feedstock sources

In this study the feedstock biomass utilized in fermentation processes is categorized under the broad term "lignocellulosic biomass." We assume that the yields for isobutanol, isobutene, and ethanol remain consistent and are not influenced by the specific type of lignocellulosic biomass employed, whether it be herbaceous crops or agroforestry residues. This assumption neglects variations in yields and process performances observed when different types of lignocellulosic biomass serve as feedstocks, as reported by Morales et al., 2021 [65].

We support this hypothesis by noting the prevalent use of corn stover (agricultural residues) in the majority of literature on life cycle assessments (LCAs), including the studies upon which we rely for ethanol and i-BuOH pathways. These studies are primarily conducted in the USA, where corn stover share in residue feedstock availability is higher than in Europe.

In contrast, the IBN-SAF supply chain hinges on the utilization of forestry residues, aligning with the REWOFUEL project's objective to assess the potential of softwood for biofuel production.

Introducing a diversification in fermentation yield for each production process would require an effort inconsistent with the goals of this thesis. Corn stover serves as a reasonable compromise in terms of chemical composition between herbaceous energy crops and residues. Therefore, we consider the yields obtained for ethanol and isobutanol pathways, using corn stover, as the average yield between those that would be obtained using switchgrass or residues. However, the yield for the IBN pathway might be enhanced if higher carbohydrate content feedstocks, such as herbaceous crops, were employed.

Furthermore, leveraging on fermentation processes associated with different biomass types would not significantly impact overall emission of the well-to-wings analysis. This happens since we have considered the specific emissions from biomass farming and collection processes related to different biomass types, for which we possess accurate data.

<u>Energy and Carbon balances</u>

The evaluation of environmental sustainability in the production of biofuels from lignocellulosic biomass relies significantly on energy and carbon balances. These metrics play a crucial role in conducting comparisons across various supply chains. The assessment entails quantifying the energy and mass inputs and outputs across the entire conversion process, considering each stage from the sourcing of biomass feedstock to the final production of Sustainable Aviation Fuel through diverse Alcohol-to-Jet pathways. As the routes differ primarily in the industrial conversion process, while the upstream supply of lignocellulosic biomass is shared among them, the thesis will specifically outline the computation of energy and carbon balances concerning the industrial conversion process from biomass to SAF. The energy balance calculation consists of dividing the sum of the energy output (SAF, other biofuels, electricity) to the sum of the energy input (Processed biomass, electricity, natural gas, hydrogen) along the entire industrial SAF supply chain. Instead, the carbon balance computation consists of the ratio between the carbon

output to the carbon input, which is performed by using the carbon concentration of mass flows involved in the conversion process.

Table 3.11 presents the values of Lower Heating Value (LHV), density, and carbon concentration for the primary mass streams participating in the Sustainable Aviation Fuel (SAF) supply chains. These values are employed to calculate the energy and carbon balance of these streams.

Table 3.1: LHV, density and carbon content of primary energy mass stream involved in the SAF production

Name	LHV [MJ/kg]	Density [kg/m³]	C Content [%]	Ref.
Ref. biomass	15.8	60	40	[65]
Isobutanol	33.3	802	65	[83]
Ethanol	26.7	789	52	[83]
Isobutene	45.1	605	85.7	[83]
Diesel	42.6	846	87	[84]
Heavy oil	39.0	980	85	[84]
Gasoline	43.4	737	90	[84]
SAF	44.0	821	82	[85]
Natural gas	47.1	0.777	75	[84]
Hydrogen	120.0	0.09	/	[83]
Lignin	22.8	1400	66	[65]

3.1.3 Transportation from biorefinery to the airport

In order to evaluate the influence of transportation influenced by country-specific factors like size and aviation industry development, this thesis relies on EUROCONTROL's study. Conducted through its Statistics and Forecast Service (STATFOR), the study offers various air traffic forecasts for the European Air Network [86]. The intention of this source is to offer accessible and informative insights into the functioning of the air traffic industry. Despite being primarily based on 2006 data, the study notes that the lessons it imparts about airports, both large and small, remain relevant over time. Further details regarding the calculations and assumptions made in this thesis are provided in the Appendix.

3.2 Scaling-Up for meeting jet fuel demand and reducing emissions

In the analysis, simulations were conducted to explore the potential scaling-up of the different scenarios aimed at meeting jet fuel demand and reducing global emissions in European countries.

Data regarding the country-specific aviation fuel demand were acquired from The U.S Energy Information Administration. Their database encompasses information on various refined petroleum products spanning the years 1980 to 2021 [87]. Anticipating a return to pre-pandemic levels by 2025 [4], the data for the year 2019 was utilized to assess the current consumption of jet fuel for each European country. Subsequentially, the analysis focused on determining the potential coverage of jet fuel demand on a country-by-country basis. This involved incorporating SAF, derived from residues and energy crops, as a substitute for traditional aviation fuel. The assessment took into account the expectation that demand for European aviation fuel will not increase substantially after the return to pre-pandemic levels. This expectation is supported by compensatory measures implemented by air traffic management (ATM) and on advances in aircraft technology [88]. By examining the country-specific yearly potential production of sustainable aviation fuel produced through the best conversion pathway evaluated for each lignocellulosic feedstock, it became possible to calculate the projected share of replacing conventional aviation fuel with SAF. Consequently, this calculation provided insights into the potential reduction of carbon emissions associated with the adoption of biofuel.

Figure 3.9: Jet fuel demand by region and estimation up to 2050 [88]
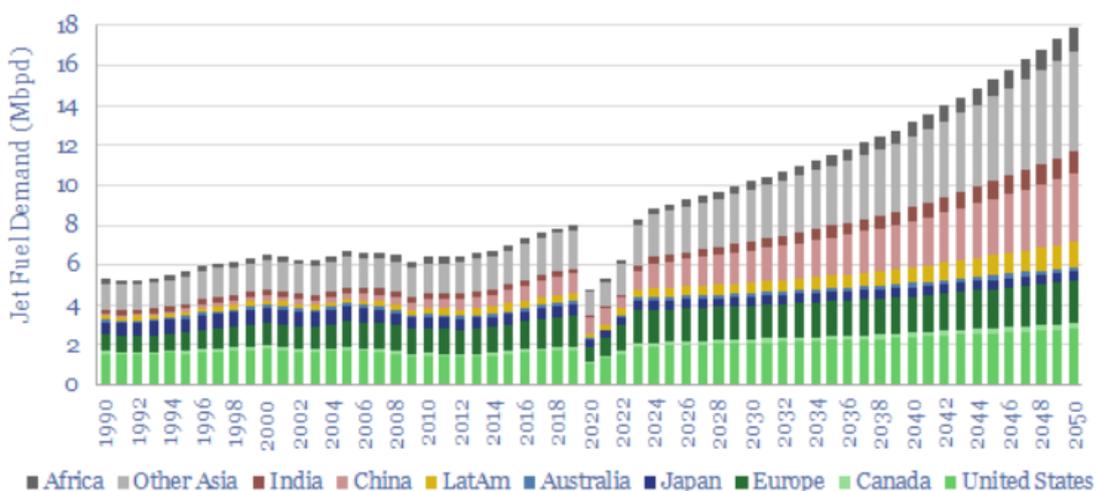
3.3 Life cycle assessment

Life Cycle Assessment (LCA) is a systematic and comprehensive method used to evaluate the environmental impacts of a product, process, or activity throughout its entire life cycle. The life cycle encompasses all stages, from the extraction of raw materials, through production and use, to disposal or recycling. The procedural structure for conducting LCA has been established as a standard by the International Organization for Standardization (ISO) under ISO 14040 and ISO 14044 (2006). This framework encompasses four key phases, visually represented in the figure: goal and scope definition, inventory analysis, impact assessment, and interpretation [89] [90] [91].

- Goal and Scope Definition: Clear outlining of the intended application, context, and modeling specifications of the analysis. These modeling specifications include specific details like the functional unit, system boundary, allocation procedure, and the environmental impacts being taken into account.

- Life Cycle Inventory (LCI): Creating a system flow model to identify and measure all inputs (e.g., materials, energy) and outputs (e.g., emissions, waste) linked to each stage of a product life cycle. These values are adjusted according to the chosen functional unit. This stage allows to build a detailed inventory outlining the resources used and environmental releases at each phase of the supply chain. The complexity of a LCA is particularly pronounced during this phase.

- Life Cycle Impact Assessment (LCIA): Evaluating the environmental impacts identified in the inventory analysis through categorization, quantification, normalization to reference values, and optional assignation of importance factors based on societal values (Weighting). This phase offers a thorough assessment of the potential environmental consequences of a product or process, contributing to a better understanding and prioritization of various impact categories.

- Interpretation: Analyzing Impact Assessment results to identify errors and data quality issues highlighted in the Inventory Analysis. After making

improvements, the LCA calculations are rerun, refining the assessment with each iteration. The discussion of results includes evaluating contributions, relevance, robustness, and limitations, systematically exploring opportunities to mitigate negative environmental impacts without burden shifting between categories or phases.

Figure 3.10: Life cycle assessment phases [91]
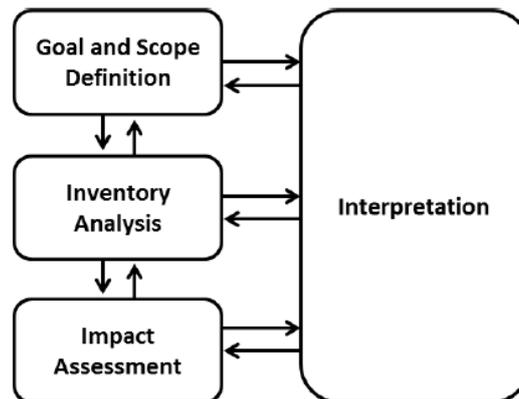
3.2.1 Goal and scope definition

This study aims to investigate the well-to-wings environmental impact of Sustainable Aviation Fuels, dealing with various process and feedstock options. The feedstocks considered are agricultural and forestry residues and herbaceous perennial energy crops suitable for the European context: Switchgrass, Reed canary and Miscanthus. The ATJ pathway has been selected to convert the chemical intermediates, produced by fermentation of feedstocks, into Synthetic Paraffinic Kerosene.

The main focus of this study is on the impact category of global warming potential over 100 years (GWP100) and the functional unit selected for this project is 1 MJ of SAF burned in an aircraft. The emission baseline for conventional aviation fuel that we consider in this analysis is set to 94 gCO_2eq/MJ, as specified in the directive EU RED 2018/2001/EC Annex V C 19 [92].

This study explores and analyzes six scenarios, each corresponding to different feedstocks and process routes and represented in Figure 3.10.

Figure 3.11: Graphical representation of the six scenarios analyzed in this study
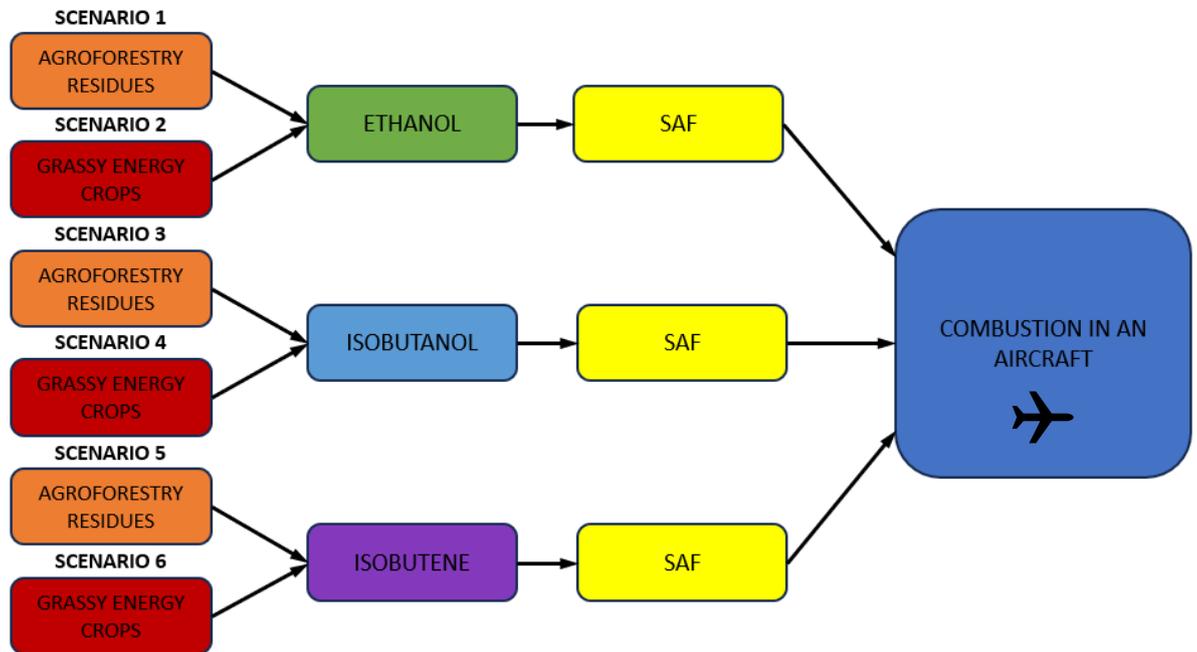
The system boundary for this assessment is illustrated in Fig. 3.11. From this boundary, it can be seen that the major stages included are: biomass production and transport, fermentation to alcohol/chemical intermediates, processing to fuel (ATJ), fuel distribution, and fuel combustion. Transportation is also included along the supply chain. Furthermore, it is assumed that the alcohol production and ATJ facilities are co-located.

Figure 3.12: System boundary for "well-to-wings" SAF supply chain, based on lignocellulosic feedstock
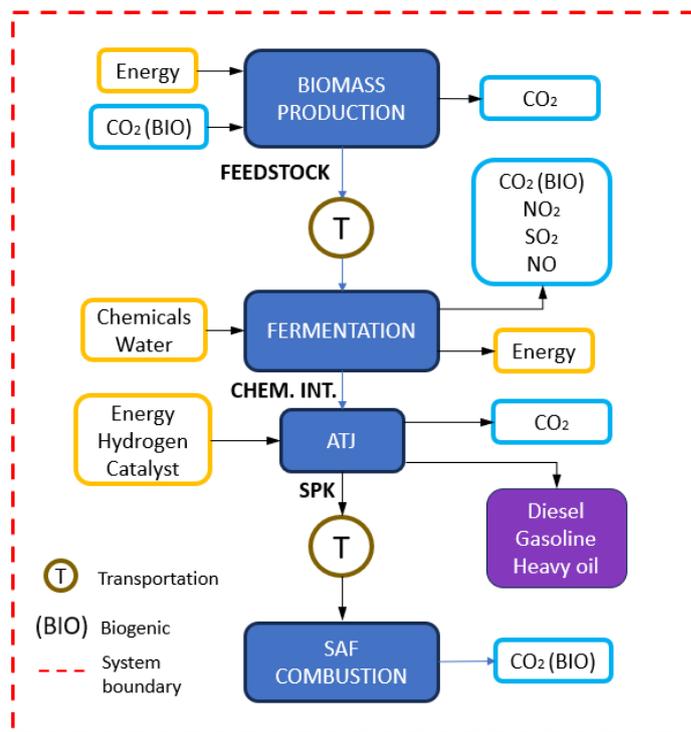
In order to evaluate the impact per 1 MJ of fuel used in an aircraft, an Excel computational sheet was developed, outlining five distinct steps for each ATJ pathway: 'Biomass production' (applicable only to scenarios involving herbaceous energy crops), 'Biomass transportation', 'Industrial conversion without electricity', 'Electricity from the grid', and 'SAF transportation'. The separation of 'Electricity from the grid' from 'Industrial conversion' aims to account for variations in the country energy mix for electricity production. In fact, the emissions from average electricity generation on the public grid vary significantly between countries, potentially leading to misinterpreted results in terms of GHG emissions. The higher the country-specific ecological electricity footprint, the greater the GHG emissions in SAF production, resulting in lower savings. For instance, the Estonian carbon footprint of the public grid is 863 gCO_2eq/kWh, while the Austrian and French footprints are 317 gCO_2eq/kWh and 76 gCO_2eq/kWh, respectively. Within the Excel model, we documented the country-specific emissions associated with each step in the SAF supply chain from ATJ pathways. The cumulative contribution of these steps yields the total carbon emissions throughout the SAF life cycle, from well-to-wings.

3.2.2 Life cycle inventory, LCI

The inventory analysis focused solely on the industrial conversion steps, as data for biomass conversion and transportation were sourced from other literature references [50] [51].

The inventories were collected for all the steps from the chipping of biomass to the final production of SAF and are grouped into 10 different datasets. These tables include the activity name, reference product, amount, unit and production location based on data from a set of sources and Ecoinvent 3.9 database. To specifically assess mass flows linked to the input used for producing 1 MJ of SAF, energy allocation was implemented. This involved rescaling all inputs according to the share of energy attributed solely to the SAF output compared to the other by-products and co-products. Employing these inventories, emissions associated with the industrial conversion step were calculated using Brightway2, a software framework designed for LCA and environmental impact analysis.

<u>Chipping and storage</u>

Table 3.2: Chipping and storage inventory to produce 1 kg of chipped biomass [65]

Name	Reference product	Amount	Unit	Location	Type
Chipping and storage	*Chipped feedstock*	*1*	*kilogram*	RER	*production*
market group for electricity, medium voltage	electricity, medium voltage	4,00E-02	kWh	RER	technosphere
market for lubricating oil	lubricating oil	2,18E-05	kilogram	RER	technosphere
market for agricultural machinery, unspecified	agricultural machinery, unspecified	1,76E-05	kilogram	GLO	technosphere

The area designated for storage and chipping manages the reception of incoming biomass feedstocks. The equipment utilized for storage and chipping is situated physically at the bioethanol plant, adjacent to the pretreatment process. Within this designated area, the biomass undergoes preprocessing and homogenization to achieve a consistent particle size and bulk density. The biomass is milled to attain a mean particle size of 40 mm. The calculations include electricity, short-time yard storage, milling, conveyor belts and for feeding biomass to the pretreatment reactor [65].

i-BuOH production via fermentation

Table 3.3 provides a compilation of the essential parameters linked to the conversion stage from lignocellulosic biomass to 1 MJ of isobutanol, based on Tao et al. [28]. It was assumed that the process plant does not produce any liquid co-products. Consequently, the data were extracted directly from the respective study, which already applies energy allocation for the different outputs. Tables 3.4 and 3.5 present the inventories related to enzyme production (i-BuOH) and corn steep liquor production, essential for the computation of the i-BuOH production inventory [28] [65].

Table 3.3: i-BuOH production via fermentation [28]

Activity name	Reference product	Amount	Unit	Location	Type
iBuOH production via fermentation	*iBuOH >99%*	*1*	*megajoule*	*RER*	*production*
Chipping and storage	Chipped feedstock	0,1442	kilogram	RER	technosphere
market for sulfuric acid	Sulfuric acid	3,26E-03	kilogram	RER	technosphere
market for ammonia, anhydrous, liquid	ammonia, anhydrous, liquid	1,73E-03	kilogram	RER	technosphere
Corn steep liquor production	Corn steep liquor	1,90E-03	kilogram	RER	technosphere
market for diammonium phosphate	Diammonium phosphate	2,30E-04	kilogram	RER	technosphere
market for sodium hydroxide, without water	sodium hydroxide, without water	3,72E-03	kilogram	GLO	technosphere
market for lime	Lime	1,50E-03	kilogram	RER	technosphere
Enzyme production (iBuOH)	Enzyme (iBuOH)	2,27E-02	kilogram	RER	technosphere
market for tap water	tap water	2,61E-01	kilogram	EwS	technosphere
nitrogen oxides		9,32E-04	kilogram		biosphere
Sulfur dioxide		9,60E-05	kilogram		biosphere

Table 3.4: Enzyme production (i-BuOH) [28]

Activity name	Reference product	Amount	Unit	Location	Type
Enzyme production (iBuOH)	*Enzyme (iBuOH)*	*1*	*kilogram*	*RER*	*production*
market for glucose	Glucose	1,70E-01	kilogram	GLO	technosphere
market for ammonia, anhydrous, liquid	ammonia, anhydrous, liquid	1,00E-02	kilogram	RER	technosphere
Corn steep liquor production	Corn steep liquor	1,00E-02	kilogram	RER	technosphere

Table 3.5: Corn steep liquor production [65]

Activity name	Reference product	Amount	Unit	Location	Type
Corn steep liquor production	*Corn steep liquor*	*1*	*kilogram*	*RER*	*production*
market for heat, district or industrial, natural gas	heat, district or industrial, natural gas	1,9E+00	megajoule	EwS	technosphere
market group for electricity, medium voltage	electricity, medium voltage	5,5E-03	kWh	RER	technosphere

Conversion of i-BuOH to SAF

Table 3.6 presents the input flows related to the conversion process of isobutanol to produce a functional unit of SAF. The inventory encompasses all the conversion steps such as dehydration, oligomerization, hydrogenation and distillation relative to the Gevo's process [17]. The process yields the simultaneous production of Heavy Oil and Diesel, amounting to 30 kJ MJ^{-1} and 80 kJ MJ^{-1}, respectively. As a result, the inventory was allocated based on the energy share of 1 MJ SAF produced relative to the total energy output, equivalent to 90.1%.

Table 3.6: Conversion of i-BuOH to SAF [17]

Activity name	Reference product	Amount	Unit	Location	Type
Conversion of iBuOH to SAF	*SAF (iBuOH)*	*1*	*megajoule*	RER	*production*
iBuOH production via fermentation	iBuOH >99%	9,15E-01	megajoule	RER	technosphere
market for heat, district or industrial, natural gas	heat, district or industrial, natural gas	5,41E-02	megajoule	EwS	technosphere
market for hydrogen, gaseous	hydrogen, gaseous	1,71E-04	kilogram	GLO	technosphere

Ethanol production via fermentation

In the table 3.7 the inputs associated with the production of 1 MJ of ethanol are outlined. The inventory relies on Table 3.5 to establish the corn steep liquor production, the data concerning cellulase enzyme was provided by NREL and it is documented in Tables 3.8. Table 3.9 lists the inputs for yeast production [14] [65] [93].

Table 3.7: Ethanol production via fermentation [14]

Name	Reference product	Amount	Unit	Location	Type
Ethanol production via fermentation	*Ethanol 99,5%*	*1*	*megajoule*	RER	*production*
Chipping and storage	Chipped feedstock	0,11713	kilogram	RER	technosphere
market for heat, district or industrial, natural gas	heat, district or industrial, natural gas	2,2E-03	megajoule	EwS	technosphere
Enzyme production (EtOH)	Enzyme (EtOH)	1,20E-03	kilogram	RER	technosphere
market for sulfuric acid	Sulfuric acid	3,87E-03	kilogram	RER	technosphere
Yeast production (EtOH)	Yeast (EtOH)	2,97E-04	kilogram	RER	technosphere
market for ammonia, anhydrous, liquid	ammonia, anhydrous, liquid	4,69E-04	kilogram	RER	technosphere
market for sodium hydroxide, without water, in 50% solution state	sodium hydroxide, without water, in 50% solution state	1,32E-03	kilogram	GLO	technosphere
market for lime	Lime	8,56E-04	kilogram	RER	technosphere
Corn steep liquor production	Corn steep liquor	1,47E-03	kilogram	RER	technosphere
market for diammonium phosphate	Diammonium phosphate	1,53E-04	kilogram	RER	technosphere
market for urea	Urea	2,34E-04	kilogram	RER	technosphere

Table 3.8: Enzyme production (EtOH) [93]

Name	Reference product	Amount	Unit	Location	Type
Enzyme production (EtOH)	*Enzyme (EtOH)*	*1*	*kilogram*	RER	*production*
market for ammonia, anhydrous, liquid	ammonia, anhydrous, liquid	2,00E-01	kilogram	RER	technosphere
Corn steep liquor production	Corn steep liquor	2,80E-01	kilogram	RER	technosphere
market for sulfur dioxide, liquid	sulfur dioxide, liquid	2,76E-02	kilogram	RER	technosphere
market for glucose	Glucose	4,18E+00	kilogram	GLO	technosphere
market for chemical, organic	chemical, organic	1,16E-01	kilogram	GLO	technosphere
market group for electricity, low voltage	electricity, low voltage	9,0E+00	kWh	RER	technosphere

Table 3.9: Yeast production (EtOH) [65]

Activity name	Reference product	Amount	Unit	Location	Type
Yeast production (EtOH)	*Yeast (EtOH)*	*1*	*kilogram*	RER	*production*
market for water, deionised	water, deionised	3,07E+01	kilogram	EwS	technosphere
market for ammonium chloride	ammonium chloride	0,37	kilogram	GLO	technosphere
market for sodium hydroxide, without water	sodium hydroxide, without water	2,30E-01	kilogram	GLO	technosphere
market for glucose	Glucose	1,99E+00	kilogram	GLO	technosphere
market group for electricity, medium voltage	electricity, medium voltage	7,7E-02	kWh	RER	technosphere
Ethanol		7,70E-03	kilogram		biosphere
Water		2,30E-04	cubic meter		biosphere
Carbon dioxide, non-fossil		8,78E-01	kilogram		biosphere

Conversion of EtOH to SAF

Table 3.10 summarizes the parametric assumptions for ETJ production processes entailing ethanol dehydration, oligomerization, hydrotreating, and product fractionation according to the study conducted by Han et al. [79]. The process results in the co-production of Gasoline and Diesel, totaling 212 kJ MJ^{-1} and 115 kJ MJ^{-1}, respectively. Consequently, the inventory was allocated by energy based on the energy share of 1 MJ SAF produced over the total energy output, which is equivalent to 75.4% of the overall impacts.

Table 3.10: Conversion of EtOH to SAF [79]

Activity name	Reference product	Amount	Unit	Location	Type
Conversion of EtOH to SAF	*SAF (EtOH)*	*1*	*megajoule*	RER	*production*
Ethanol production via fermentation	Ethanol 99,5%	1,1084	megajoule	RER	technosphere
market group for electricity, medium voltage	electricity, medium voltage	7,01E-03	kWh	RER	technosphere
market for hydrogen, gaseous	hydrogen, gaseous	5,08E-04	kilogram	GLO	technosphere
market for zeolite, slurry, without water	zeolite, slurry, without water	8,07E-05	kilogram	RER	technosphere

Conversion of lignocellulosic biomass to SAF (IBN route)

In this instance, the LCI was compiled using assessments and outcomes from the REWOFUEL project [81], encompassing all production stages from lignocellulosic biomass to sustainable jet fuel. The data in the inventory are organized at the process-unit level and are displayed in table 3.3. Similarly to previous cases, mass flows were allocated on an energy basis, taking into account the energy value of the by-products from the industrial process. The by-products include lignin (1.017 MJ MJ_{SAF}^{-1}), biomass output as animal feed (0.0786 MJ MJ_{SAF}^{-1}), and ethanol (0.5682 MJ MJ_{SAF}^{-1}). Hence, the energy share utilized to adjust the scale of all inputs is equal to 37.5%.

Table 3.11: Conversion to SAF (IBN route) [81]

Activity name	Reference product	Amount	Unit	Location	Type	Comment
Conversion to SAF (IBN route)	*SAF (IBN)*	*1*	*megajoule*	*RER*	*production*	*reference product*
Chipping and storage	Chipped feedstock	0,11737	kilogram	RER	technosphere	Feedstock to sugar
market for sulfur dioxide, liquid	sulfur dioxide, liquid	1,18E-03	kilogram	RER	technosphere	Feedstock to sugar
Enzyme production (iBuOH)	Enzyme (iBuOH)	4,49E-03	kilogram	RER	technosphere	Feedstock to sugar
market for sodium hydroxide, without water	sodium hydroxide, without water	3,79E-03	kilogram	GLO	technosphere	Feedstock to sugar
market for sulfuric acid	Sulfuric acid	9,84E-05	kilogram	RER	technosphere	Feedstock to sugar
market for polydimethylsiloxane	polydimethylsiloxane	4,53E-06	kilogram	GLO	technosphere	Feedstock to sugar
market for tap water	tap water	4,06E-01	kilogram	EwS	technosphere	Feedstock to sugar
treatment of wastewater, wastewater treatment	wastewater, average	2,60E-04	cubic meter	EwS	technosphere	Feedstock to sugar
market for sodium hydroxide, without water	sodium hydroxide, without water	3,25E-06	kilogram	GLO	technosphere	Fermentation
market for polydimethylsiloxane	polydimethylsiloxane	4,53E-06	kilogram	GLO	technosphere	Fermentation
market for phosphoric acid, without water	phosphoric acid, without water	8,62E-06	kilogram	GLO	technosphere	Fermentation
market for sodium chlorate, powder	sodium chlorate, powder	4,84E-04	kilogram	RER	technosphere	Fermentation
market for ammonia, anhydrous, liquid	ammonia, anhydrous, liquid	3,42E-04	kilogram	RER	technosphere	Fermentation
market for tap water	tap water	1,11E-01	kilogram	EwS	technosphere	Fermentation
treatment of wastewater, wastewater treatment	wastewater, average	1,65E-04	cubic meter	EwS	technosphere	Fermentation
market for hydrogen, gaseous	hydrogen, gaseous	3,25E-06	kilogram	GLO	technosphere	Conversion to SAF
market for isobutane	isobutane	7,52E-06	kilogram	GLO	technosphere	Conversion to SAF
market for tap water	tap water	9,30E-10	kilogram	EwS	technosphere	Conversion to SAF
market for sodium hydroxide, without water	sodium hydroxide, without water	1,48E-03	kilogram	GLO	technosphere	Off-site
market for sulfuric acid	Sulfuric acid	1,84E-04	kilogram	RER	technosphere	Off-site
market for phosphoric acid, without water	phosphoric acid, without water	1,55E-05	kilogram	GLO	technosphere	Off-site
market for nitrogen, liquid	nitrogen, liquid	5,45E-04	kilogram	RER	technosphere	Off-site
market for iron(III) chloride, without water	iron (III) chloride, without water	2,10E-05	kilogram	GLO	technosphere	Off-site
market for quicklime, milled, packed	quicklime, milled, packed	1,01E-03	kilogram	RER	technosphere	Off-site
market for tap water	tap water	7,19E-01	kilogram	EwS	technosphere	Off-site

Note: Europe (RER), Europe without Switzerland (EwS), Global (GLO)

3.2.3 Life cycle impact assessment, LCIA

This thesis employed the Brightway and Ecoinvent tools for conducting the Life Cycle Assessment (LCA). The Brightway LCA framework was facilitated by the open-source software Activity Browser, which provides a graphical user interface. Background data essential for the LCA was obtained from the Ecoinvent 3.9 and Biosphere 3 databases. These databases encompasse over 25000 activities, modeling human activities and offering detailed information on industrial and agricultural processes, including natural resource extraction, emissions to water, soil, and air, products from other processes, as well as co-products and waste [94].

When assessing the environmental impact of a project, it is important to consider various impact categories. In this particular case, significant attention was directed toward the impact category related to climate change. The selected method for impact assessment was based on IPCC 2021, specifically focusing on climate change and global warming potential, with a specific emphasis on GWP100. This metric evaluates the global warming potential of greenhouse gases over a 100-year period.

Results and discussion

This chapter presents a comprehensive review of key findings from life cycle assessment (LCA) of SAF from lignocellulosic feedstock. Initially, it examines various industrial processes, discussing yields, carbon and energy efficiency associated with producing SAF through different routes. Subsequently, the LCA results are presented, focusing on the primary impact category, climate change (GWP100). A detailed discussion is undertaken to elucidate the reasons behind observed differences among countries and pathways. Additionally, the chapter assesses the potential scalability of these systems, evaluating their capacity to meet the increasing demand for aviation fuel in European countries. The discussion extends to the emission savings achievable through widespread adoption of this innovative technology.

4.1 Yields, carbon and energy balance of conversion routes

Using the inventories specifically selected for each pathway inherent in the production of chemical intermediates and further upgrading to SAF, the relative yields of mass and energy could be evaluated. This approach allowed a comprehensive analysis of the specific characteristics of various industrial processes, highlighting their differences.

4.1.1 Yields

The Isobutene pathway demonstrates the best result in terms of feedstock demand, quantified as the allocated biomass input required per functional unit of SAF, with an assessed value of $0.117\,\mathrm{kg_{db}\,MJ_{SAF}^{-1}}$. Unfortunately, due to a lack of information on the production process for this route, the actual yield of isobutene produced from lignocellulosic feedstock and its subsequent conversion into iso-paraffinic kerosene could not be determined. Nevertheless, based on insights from existing literature, it can be inferred that given the recentness of the technology, the performance of isobutene fermentation may be comparatively lower in terms of $\mathrm{kg_{db}\,MJ_{SAF}^{-1}}$. However, the high conversion efficiency into SAF, coupled with the absence of dehydration conversion steps along the production chain, results in an overall yield that is the highest. Notably, isobutene oligomerization in this pathway does not

generate significant amounts of co-produced fuels such as gasoline or diesel, showcasing a high selectivity for SAF production. This significant achievement underscores the potential of this innovative pathway, furthering its coming inclusion in the ASTM standard specification for aviation turbine fuel containing synthesized hydrocarbons. The only by-products of the process are lignin (which exceeds the fuel demand of the CHP plant), C5 sugar (expressed as ethanol equivalent), biomass (for animal feed), and calcium (Ca) and potassium (K) as fertilizers, which can be exploited for other industrial supply chains.

Due to higher technology readiness level (TRL), the ethanol yield, evaluated in terms of kg of biofuel per kg biomass, is the highest among the pathways, with a value of 26.8%, while for isobutanol, this value was evaluated at 19.4%. However, significant differences arise when considering the conversion of alcoholic intermediates into Sustainable Aviation Fuel. In this crucial step, the SAF yield, defined as kg of SAF per kg of chemical intermediate input, stands at 74.5% and 42.1% for i-BuOH and EtOH, respectively. These variations are attributed to the higher presence of co-products in the ethanol route compared to the Isobutanol route. In fact, for every kilogram of SAF derived from the ethanol supply chain, 214g of gasoline and 93.4g of diesel are produced. In contrast, each kilogram of SAF distilled from the isobutanol conversion pathway results in the co-production of only 82.6g of diesel and 33.8g of heavy oil. These findings align with existing literature, indicating that ethylene has a tendency to form C2-C8 oligomers rather than C10+, while isobutanol oligomerization leads to higher yields in the range of kerosene oligomers. However, even after applying energy allocation, the overall feedstock demand remains more favorable for ethanol than isobutanol, with evaluated values of 0.130 kg_{db} MJ_{SAF}^{-1} and 0.132 kg_{db} MJ_{SAF}^{-1}, respectively, based on selected inventories [14] [17] [28] [65] [93]. With ongoing technological advancements and the development of engineered yeast, leading to an increase in isobutanol yield, this finding may become more favorable for isobutanol in the future as well as for isobutene.

4.1.2 Carbon balance

The carbon efficiency, calculated as the ratio of carbon mass in the output liquid fuels to carbon mass in the reference biomass, resulted in 23.9%, 30.8%, and 33.3% for the IBN, EtOH, and i-BuOH routes, respectively. Considering the studies selected in this thesis, the results remark the higher carbon efficiency of the i-BuOH supply chain in harnessing the carbon content in the feedstock to produce a chain of iso-paraffinic kerosene. The IBN route exhibits the lowest carbon efficiency due to the lower IBN yield compared to isobutanol and ethanol production. Such a lower yield signifies a reduced exploitation of the sugars contained in the lignocellulosic feedstock, resulting in a higher production of by-products such as lignin. Figures 4.1, 4.2, and 4.3 illustrate the distribution of carbon contained in the input biomass among the various by-products and co-products of the three processes. It depicts that most of the carbon is found in lignin, which is either completely or partially burned in the cogeneration plant, followed by SAF and other co-produced fuels and by-products. Table 4.1 quantifies the relative amounts of carbon expressed in kilograms for each process output and evaluated considering 100kg of chipped reference biomass.

Figure 4.1: Percent distribution of carbon in various process outputs - i-BuOH

Isobutanol route

2.60%　1.05%
29.70%
66.65%

SAF ■ Lignin burned in CHP ■ Diesel ■ Heavy oil
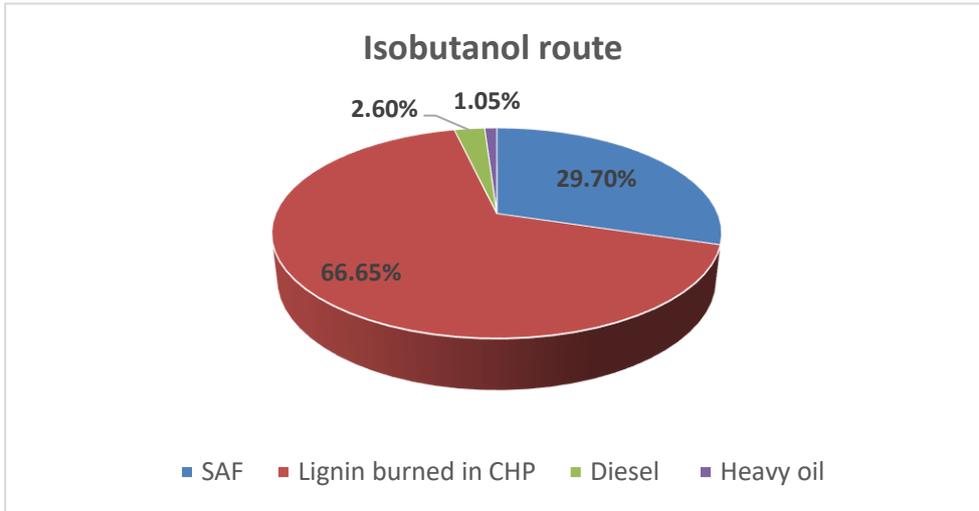
Figure 4.2: Percent distribution of carbon in various process outputs - EtOH route

Ethanol route

2.85% 5.33%
22.60%
69.23%

SAF ■ Lignin burned in CHP ■ Diesel ■ Gasoline
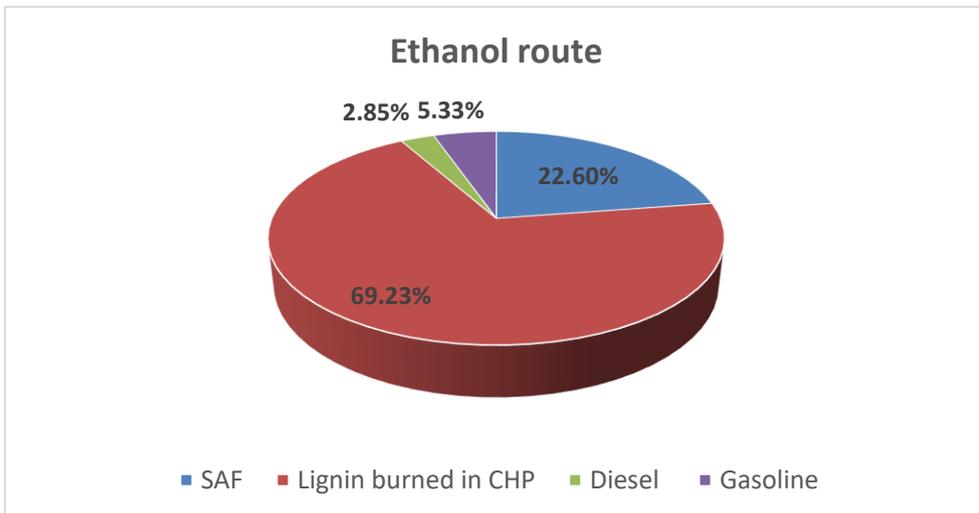
Figure 4.3: Percent distribution of carbon in various process outputs - IBN route

Isobutene route

8.88%
15.03%
16.68%
23.70%
35.73%

SAF ■ Lignin burned in CHP ■ Lignin unburned ■ Biomass ■ Ethanol
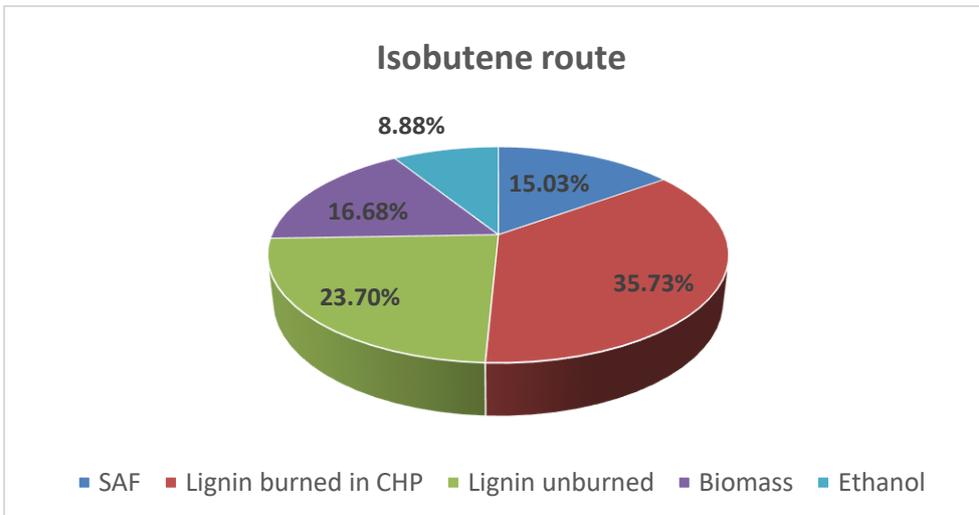
Table 4.1: Amount of carbon in various process outputs and carbon efficiency [14] [17] [28] [65] [81]

Carbon Balance			
Process output	i-BuOH route	EtOH route	IBN route
	[kg]	[kg]	[kg]
Lignin burned in CHP	26.66	27.69	14.29
SAF	11.88	9.04	6.01
Gasoline	-	2.13	-
Diesel	1.04	1.14	-
Heavy oil	0.42	-	-
Lignin unburned	-	-	9.48
Biomass	-	-	6.67
Ethanol	-	-	3,55
Total Carbon (ref. Biomass)	40	40	40
Carbon efficiency	33.3%	30.8%	23.9%

4.1.3 Energy balance

The energy efficiency of each pathway was evaluated by considering all energy flows across the system boundary, including electricity, natural gas, hydrogen, co-products and by-products. Energy efficiencies of 42.4%, 46.2%, and 47.5% were determined for ethanol, isobutanol, and isobutene, respectively. The higher energy efficiency in the i-BuOH route compared to the EtOH route can be attributed to the lower amount of hydrogen required for the industrial process, reflecting higher industrial efficiency in converting alcohol into Sustainable Aviation Fuel. Specifically, for 100 kg of chipped biomass input, the hydrogen demand is 0.121 kg for the isobutanol pathway and 0.326 kg for the ethanol pathway. Both i-BuOH and EtOH fermentation processes generate surplus electricity in the Combined Heat and Power plant, with a slightly higher value for the ethanol route (51 MJ versus 47 MJ). Natural gas and electricity are utilized in SAF conversion steps to meet the process heat demand, with values of 38 MJ of natural gas used in the isobutanol route and 16 MJ of electricity used in the ethanol route. To remind, the electricity required for the ethanol production plant is supplied from the grid electricity, owing to the chosen standalone configuration of production plants. As technology progresses, the development of an integrated plant that combines fermentation and conversion to SAF plants, similar to what was contemplated for the IBN route, has the potential to decrease external energy demand, thereby boosting overall energy

efficiency. The overall energy output due to liquid fuels from industrial processes favors the i-BuOH pathway, totaling 707 MJ compared to 642 MJ for the ethanol one.

The IBN supply chain stands out for its superior energy efficiency, despite its high electricity requirement (224 MJ) for the conversion process, which ranks it with the highest energy input among all those considered.

The primary driver of this good performance is the significant energy contribution of by-products of such pathway, especially unburned lignin, followed by ethanol and biomass. Another reason may be sought the lower requirement of hydrogen to transform isobutene into SAF, which is 2.78 g and the additional input of 5.41 g of isobutane per 100 kg of biomass input, according to Puschnigg et al. [81]. The minimal mass demand results in an almost negligible contribution to the overall energy balance. The detailed explanation for the minimal hydrogen quantity and the supplementary input of isobutane in the IBN supply chain was not extensively discussed in the available literature sources, as the process details are safeguarded due to the sensitivity of the technology involved. Another contributing factor to the superior energy efficiency of the IBN configuration facilities is the assumption of integrated plants, leading to a more effective exploitation of energy fluxes within the system boundary. This characteristic positions the IBN route leading to higher energy-efficient process among the selected studies for SAF pathways, despite its drawback of having a lower carbon efficiency due to lower biofuel yields.

The findings, based on a reference biomass input of 100 kg, are outlined in Table 4.2. It is evident that the primary energy input for the processes is attributed to the reference biomass (1580 MJ), while the energy impact of electricity and conversion-related chemicals, such as natural gas and hydrogen, remains relatively low. Figures 4.4, 4.5, and 4.6 visually depict the distribution of output energy streams in the SAF supply chains. It is apparent from these figures that, when considering an equal amount of reference biomass and without accounting for energy allocation, the i-BuOH route achieves the highest iso-paraffinic kerosene yield, equal to 84%. However, the isobutene route, despite yielding the highest overall energy outputs, it exhibits the lowest share of SAF produced from the supply

chain, totaling approximately 38%. This indicates a limitation in its capacity to generate a substantial amount of bio jet fuel from the same lignocellulosic biomass. However, it is crucial to emphasize that the by-products generated in the value chain, including lignin, ethanol, sludge, and microbial biomass, are valuable resources. They possess significant energy value and can find applications across various industries. Finally, Table 4.7 summarizes and compares the energy and carbon efficiencies evaluated in this study.

Table 4.2: Main energy inputs and outputs for the different supply chains [14] [17] [28] [65] [81]

Energy Balance			
	i-BuOH route	EtOH route	IBN route
	[MJ]	[MJ]	[MJ]
Process inputs			
Reference Biomass	1580	1580	1580
Electricity from the grid	-	16.2	224.0
Natural gas	38.2	-	-
Hydrogen	14.5	39.1	n.r.
TOTAL	1632.7	1635.3	1804.0
Process outputs			
Co-produced eletricity	47.0	51.4	-
SAF	637.6	484.2	322.5
Gasoline	-	102.7	-
Diesel	51.0	55.7	-
Heavy oil	19.1	-	-
Lignin unburned	-	-	326.7
Ethanol	-	-	181.8
Biomass	-	-	25.2
TOTAL	754.7	694.0	856.2
Energy efficiency	46.2%	42.4%	47.5%

Figure 4.4: Energy share of different output streams - i-BuOH route

Isobutanol route

6,8% 2,5% 6,2%

84.5%

■ Co-produced eletricity ■ SAF ■ Diesel ■ Heavy oil
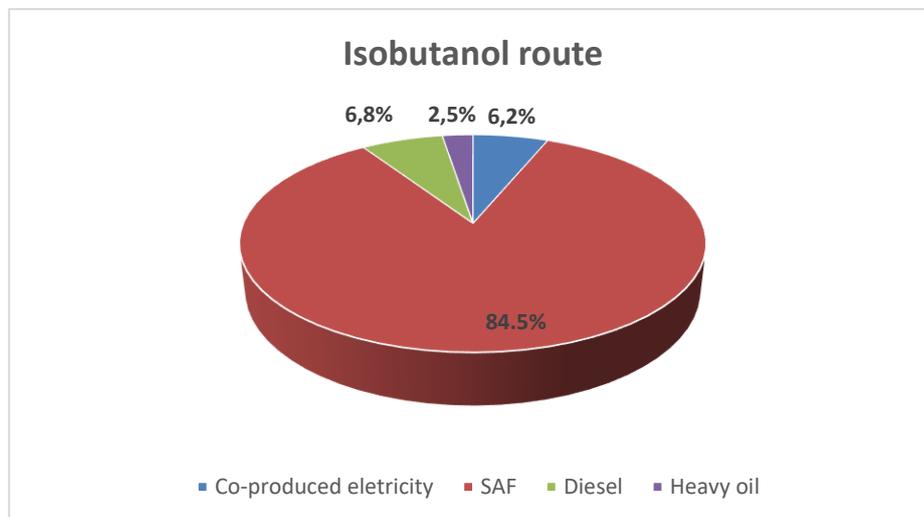
Figure 4.5: Energy share of different output streams - EtOH route
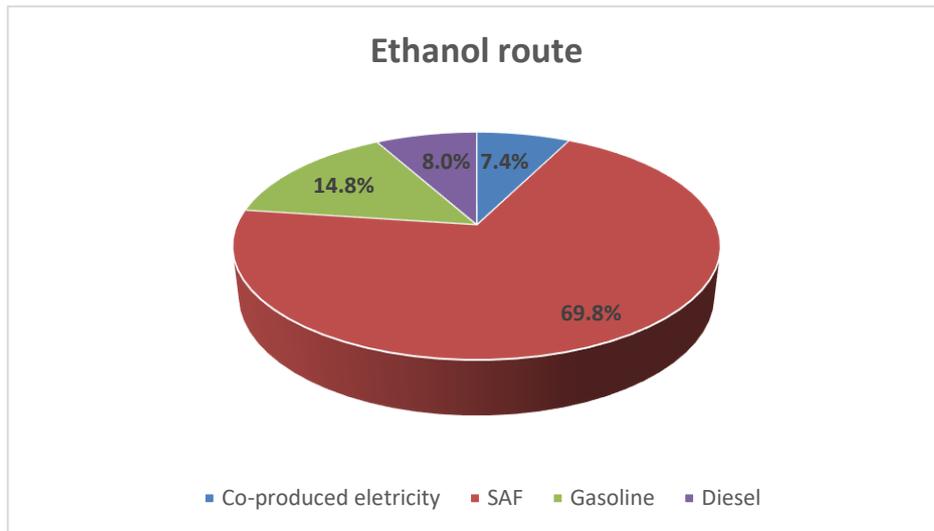
Figure 4.6: Energy share of different output streams - IBN route
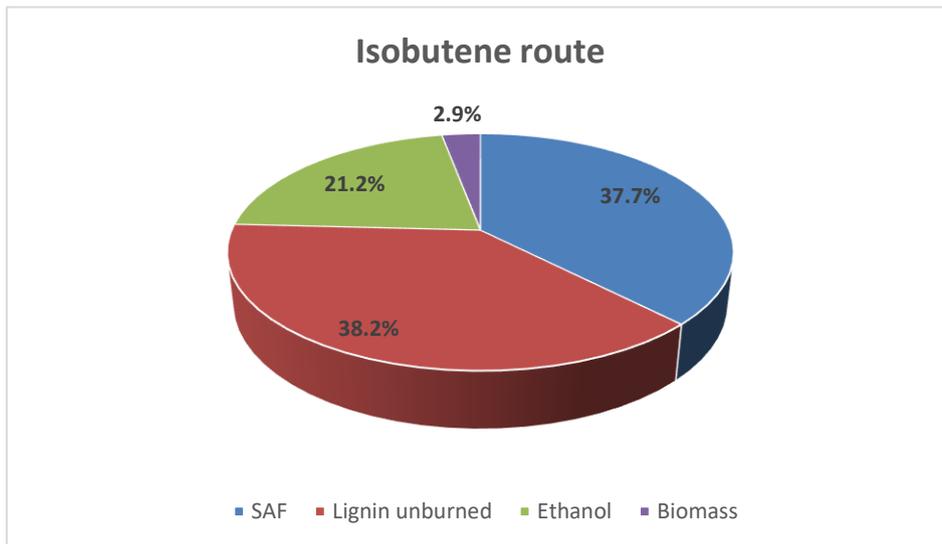
Figure 4.7: Comparation of Carbon and energy efficiency of the different routes
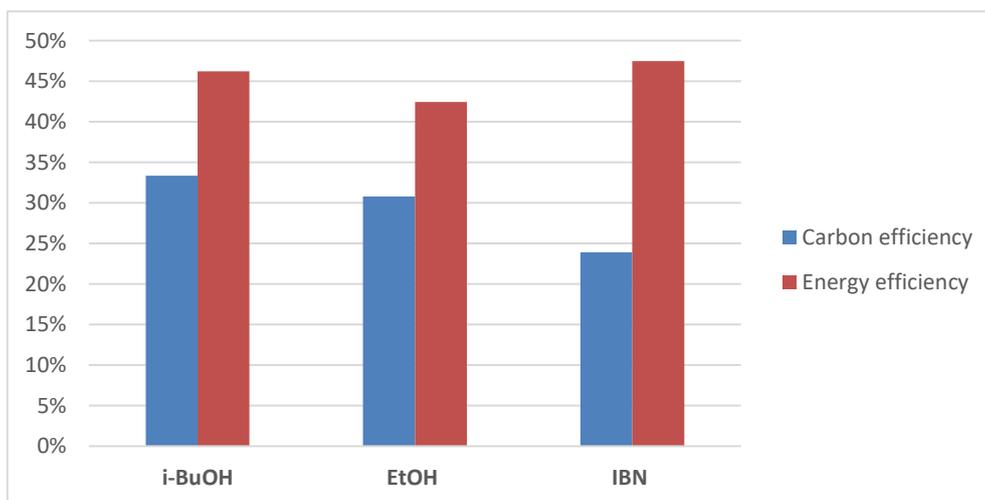
4.2 Global Warming Potential (GWP100)

Using the compiled inventories, a life cycle assessment was performed to evaluate the environmental impact of the scenarios examined. The LCA results were used to determine the emissions associated with the industrial conversion process in the production of SAF through various technologies, excluding electricity. Graphical representations offer a visual understanding of the main factors shaping life cycle emissions in different supply chains and they specifically highlight the principal contributors driving the overall production emission.

Figures 4.8, 4.9 and 4.10 show the country-based GHG intensities of EtOH, i-BuOH and IBN route respectively to produce SAF from herbaceous energy crops such as Switchgrass, Reed Canary and Mischanthus, whereas figures 4.11, 4.12, and 4.13 present the same supply chains, focusing on the exploitation of agroforestry residues. The results are presented country-by-country and as European average, highlighting the baseline of conventional aviation fuel that is set at 94 gCO_2eq/MJ and are first discussed on conversion step basis during the next paragraphs. Due to the extensive amount, the numerical results of emissions referred to each step and to each country, are mainly reported in the tables present in the appendix of the thesis.

4.2.1 Biomass production

Concerning the herbaceous energy crops cultivations (bioenergy crops cultivated in abandoned cropland areas), Switchgrass demonstrates the highest suitability for the agroclimatic conditions in European countries, emerging as the most favorable option for 24 out of 28 countries [51]. In contrast, Reed Canary exhibits compatibility with Norway and Finland, and Miscanthus is the best choice only for Portugal. On the other hand, when considering emissions associated with biomass production, Miscanthus proves to be the most favorable, with approximately 133 gCO_2eq kg_{db}^{-1}. In comparison, Switchgrass and Reed Canary show emissions of 162.9 gCO_2eq kg_{db}^{-1} and 187.6 gCO_2eq kg_{db}^{-1}, based on the study of Gvein et al. [79].

Biomass production significantly contributes to the overall life cycle emissions in all sustainable aviation fuel (SAF) supply chains.

However, the absolute contribution varies based on the feedstock demand and the type of biomass feedstock employed in the production route. Despite differences in feedstock demand among various conversion processes, the overall impact is not highly significant on average. For instance, with Switchgrass, the emissions range from 19.1 gCO_2eq MJ_{SAF}^{-1} for the isobutene route to around 21 gCO_2eq MJ_{SAF}^{-1} for the isobutanol and ethanol routes. In contrast, when Miscanthus cultivation is evaluated, it results in lower emissions, varying from 17.3 gCO_2eq/MJ_{SAF} to 17.6 gCO_2eq MJ_{SAF}^{-1}. Finally, Reed Canary cultivation has the highest impact, with emissions assessed at 22 gCO_2eq MJ_{SAF}^{-1}, 24.4 gCO_2eq MJ_{SAF}^{-1}, and 24.8 gCO_2eq MJ_{SAF}^{-1} per IBN, EtOH, and i-BuOH, respectively. The results of biomass emission related to the functional unit are illustrated in Table 4.5.

Hence, the impact of biomass production comprises a substantial portion of the overall life cycle emissions in supply chains utilizing herbaceous energy crops. This impact varies, representing from 33.9% in Luxembourg to 49.2% in France for the ethanol pathway, 37.8% in Luxembourg to 49.1% in France for the isobutanol pathway, and ranging from 17.5% in Poland to 52.1% in Switzerland for the isobutene pathway. The higher share in France and Switzerland is primarily attributable to lower conversion emissions owing to reduced electricity-associated emissions in these countries. This phenomenon elevates the proportion of biomass production emissions in the overall emissions. However, a more detailed discussion on the reasons for these lower emissions will be provided later.

Table 4.3: Emission associated to various herbaceous feedstock and route, expressed per functional unit

Energy Balance		
i-BuOH route	**EtOH route**	**IBN route**
$[gCO_2eq/MJ_{SAF}]$	$[gCO_2eq/MJ_{SAF}]$	$[gCO_2eq/MJ_{SAF}]$
Mischantus 17.3	17.6	15.7
Switchgrass 21.1	21.5	19.1
Reed canary 24.4	24.8	22.0

As previously detailed in the methodology chapter, emissions associated with biomass cultivation in the context of agroforestry residues are intentionally omitted from this analysis. This exclusion is due to the complete allocation of such emissions to the primary product of the crop (e.g., wheat, rye, barley, oats, maize, rice, rapeseed, and sunflower). Additionally, data pertaining to biomass collection has been disregarded, as its contribution was deemed negligible in the overall analysis.

4.2.2 Biomass transportation to Biorefinery facilities

Biomass transport emissions exhibit variability based on the availability of herbaceous crops and agroforestry residues in different European countries, considering optimal distances from fields to biofuel plants with a capacity of 560 $kton_{db}$ $year^{-1}$. In terms of the functional unit, the emissions linked to transportation to biorefinery plants for each country are presented with the reference of i-BuOH route, as the results are remain consistent also for the other pathways. The emissions range between 1 gCO_2eq MJ_{SAF}^{-1} for Lithuania and around 15 gCO_2eq MJ_{SAF}^{-1} for Finland. This signifies a negligible contribution for Lithuania and a substantial one for Finland, impacting overall emissions by approximately 22% in the worst-case scenario. The differences are attributed to the uneven distribution of resources among countries, discussed further in the Appendix.

Regarding agroforestry residues, similar considerations apply. Again, concerning the functional unit, the emissions related to transportation to biorefinery plants for each country are assessed. Minimum values are observed for Denmark, approximately 0.7 gCO_2eq MJ_{SAF}^{-1}, and maximum values for Norway, around 3 gCO_2eq MJ_{SAF}^{-1}. The reason why, even in the worst-case scenario, the overall emissions contribution is significantly lower than in previous cases with herbaceous feedstock can be attributed to the overall higher distribution of residues production across various countries, as presented in the Appendix. This superior distribution results in shorter transportation distances, making the impact less significant. Figure 4.8 and 4.9 present the country-based transport emissions per functional unit, with reference to the i-BuOH pathway.

Figure 4.8: Country-based emissions related to transportation of herbaceous biomass - i-BuOH route

Transport emissions - Herbaceous energy crops
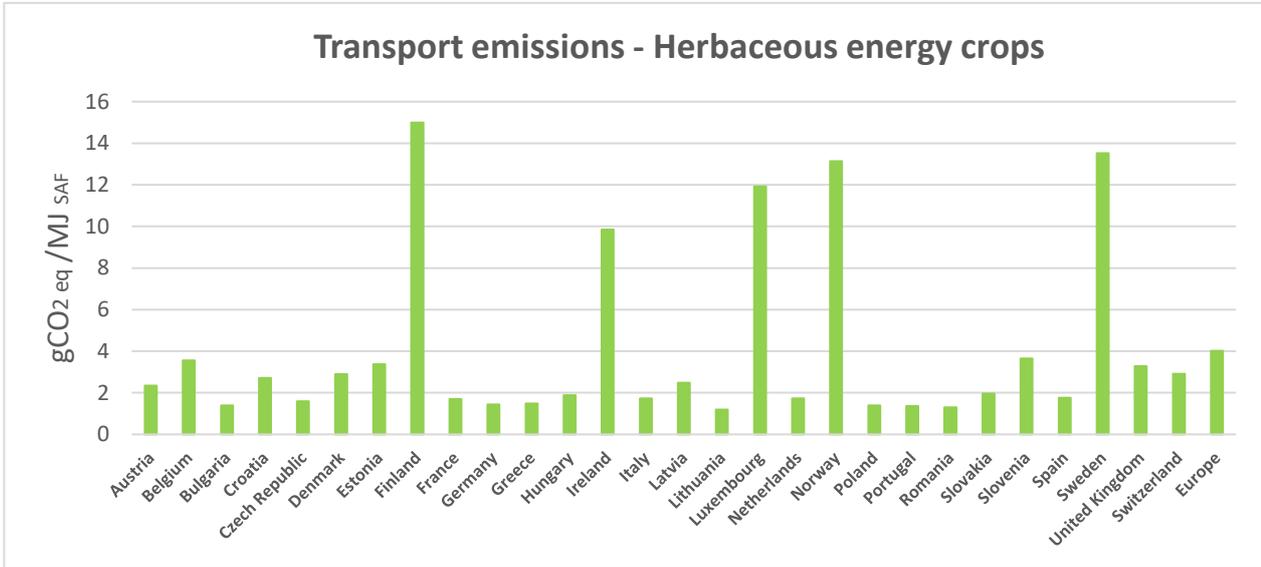
Figure 4.9: Country-based emissions related to transportation of residues - i-BuOH route

Transport emissions - Residues
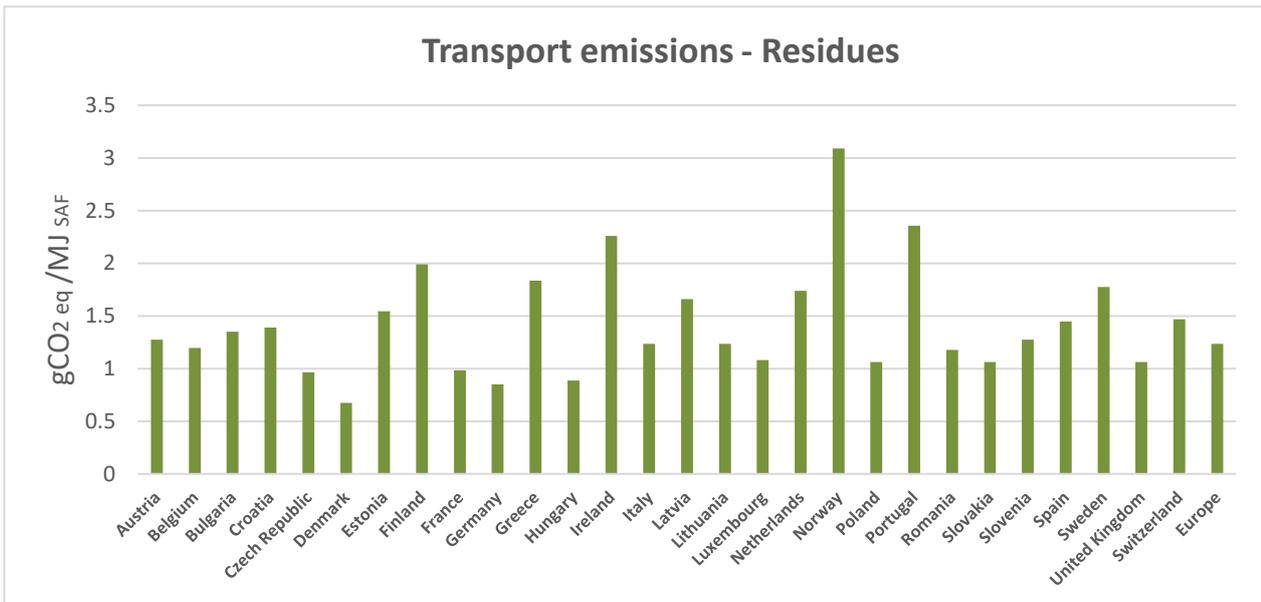
4.2.3 Industrial conversion into SAF

The process of industrial conversion encompasses all the stages from biomass chipping to the transformation into iso-paraffinic kerosene. Within the same supply chain, the primary factor influencing emission disparities among European countries is the carbon intensity of electricity generation, determined by the electricity mix of each national grid. Conversely, emissions associated with chemicals and other inputs in the conversion process are assumed to be consistent

across all countries. In order to address this effect, the life cycle assessment (LCA) conducted using Brightway2 employed inventories that excluded electricity demand. The Excel computation sheet, presented in the Appendix, delineates two distinct columns to categorize industrial conversion emissions without electricity (uniform across all countries and feedstock types) and emissions linked to electricity (varying based on each country's electricity mix). The following paragraphs will present and discuss the results of both categories.

Industrial conversion without electricity

When addressing the impact of chemicals, it incorporates all chemical inputs throughout the entire process, which includes steps such as chipping, enzyme and yeast production, fermentation, and the process of transformation into SAF. Based on this premise, the carbon emissions per functional unit, as depicted in Figure 4.10, were determined to be 15 and 17.9 gCO_2eq MJ_{SAF}^{-1} for the fermentation step to produce ethanol and isobutanol, respectively. Considering the overall production chain from reference biomass to SAF, the emissions were found to be 12.5 gCO_2eq MJ_{SAF}^{-1}, 18.1 gCO_2eq MJ_{SAF}^{-1}, and 19.8 gCO_2eq MJ_{SAF}^{-1} for the IBN, EtOH, and i-BuOH routes, respectively, as illustrated in figure 4.11. Notably, the higher carbon footprint associated with isobutanol production compared to ethanol persists even after implementing the SAF conversion step. However, the additional contribution from this step is lower for the i-BuOH route (1.9 gCO_2eq MJ_{SAF}^{-1}) compared to the EtOH route (3.1 gCO_2eq MJ_{SAF}^{-1}). It is important to consider that, for the ethanol route, the industrial process to convert EtOH to SAF requires a certain amount of electricity to cover the heat demand, whereas for the i-BuOH route, additional electricity is not used. This is because natural gas is utilized to meet the heat demand, and natural gas is already included in the inventory according to the simulations from CORSIA [17]. The superior emission performance of i-BuOH compared to EtOH in converting the chemical intermediate into SAF aligns with the earlier discussion regarding the higher SAF yields of the former process. The higher the yield, the lower the emissions associated with 1 MJ of SAF, as they depend mainly on the amount of hydrogen needed for oligomers hydrogenation, which is lower for the i-BuOH supply chain compared to the EtOH one.

Regarding the IBN route, although analogous considerations cannot be made due to the grouping of processes in one main inventory, it is evident that, excluding the high electricity demand, this supply chain exhibits the lowest emissions associated with chemical inputs. This observation can be attributed to the allocated yield, which was found to be the highest in the IBN pathway, resulting in lower amounts of chemicals per functional unit and lower feedstock consumption per megajoule of SAF produced.

Figure 4.10: Emissions per functional unit related to alcohols industrial production without electricity
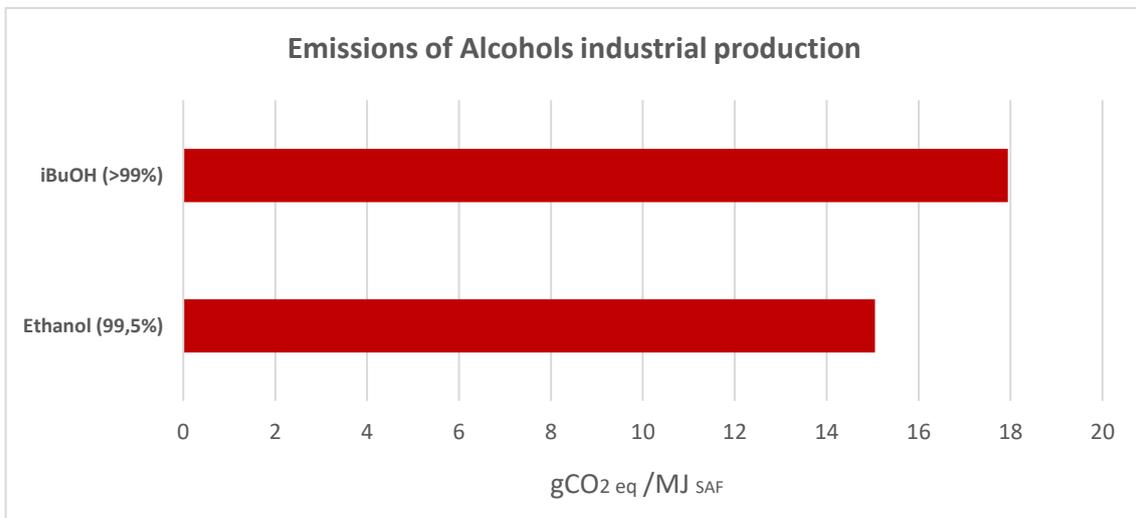
Figure 4.11: Emissions per functional unit related to SAF industrial production without electricity
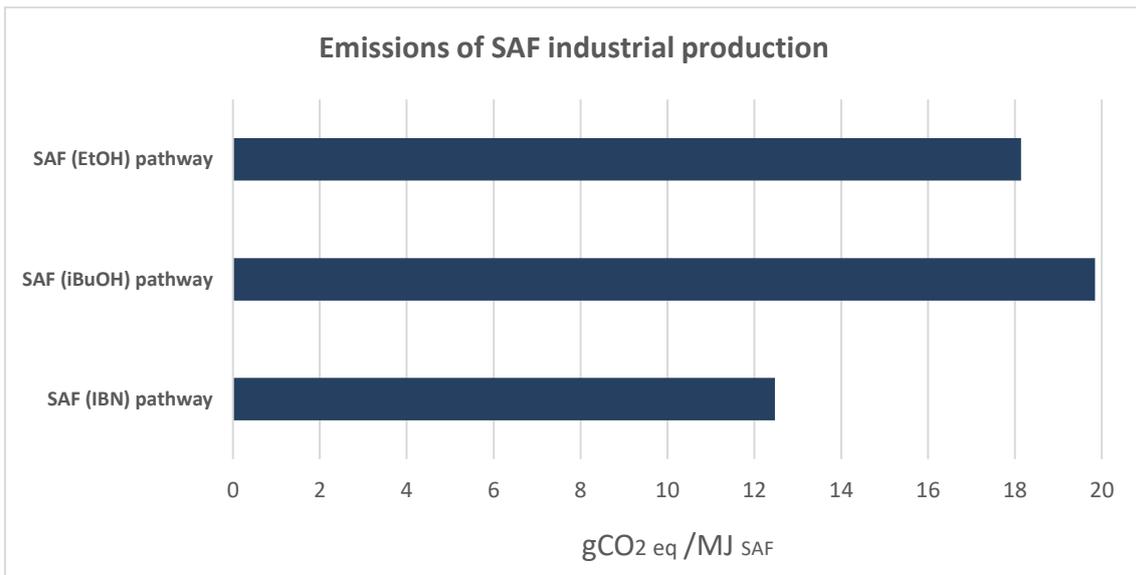
When dealing with multiple inventories and inputs in an industrial process, Sankey diagrams are useful in visualizing the main percentage contributors to overall emissions. In Figures 4.11 and 4.12, segments of the Sankey diagrams for the isobutene and ethanol pathways are presented, revealing the contributions of key impacts.

In the Sankey diagram for SAF production through isobutanol, the enzyme emerged as the largest contributor, accounting for 33%, followed by ammonia at 22%, sodium hydroxide at 22%, and natural gas at 15%. Contrasting percentages were observed for the ethanol route, where enzyme constituted 57%, sodium hydroxide 10%, ammonia 8%, yeast 7%, and hydrogen 7%. The predominant impact in terms of percentage was attributed to the enzyme, aligning with existing literature that emphasizes the significance of enzymes, which can vary based on the type of enzyme used and the pretreatment method. In this study, only the enzyme used for ethanol production (cellulase) is specifically known, while for isobutanol and isobutene production, only the enzyme inventory was provided. According to other sources, cellulase may exert a substantial impact in terms of emissions per unit of fuel produced, often due to its higher required quantity compared to other enzymes. Additionally, the higher percentage contribution of enzyme in the ethanol route can be explained by the greater electricity demand in this pathway compared to the i-BuOH route, where natural gas is utilized instead. The exclusion of electricity in this simulation amplifies the share of other inputs, further emphasizing the significance of enzyme in the overall emissions profile.

Figure 4.12: Sankey diagram of emissions - i-BuOH route
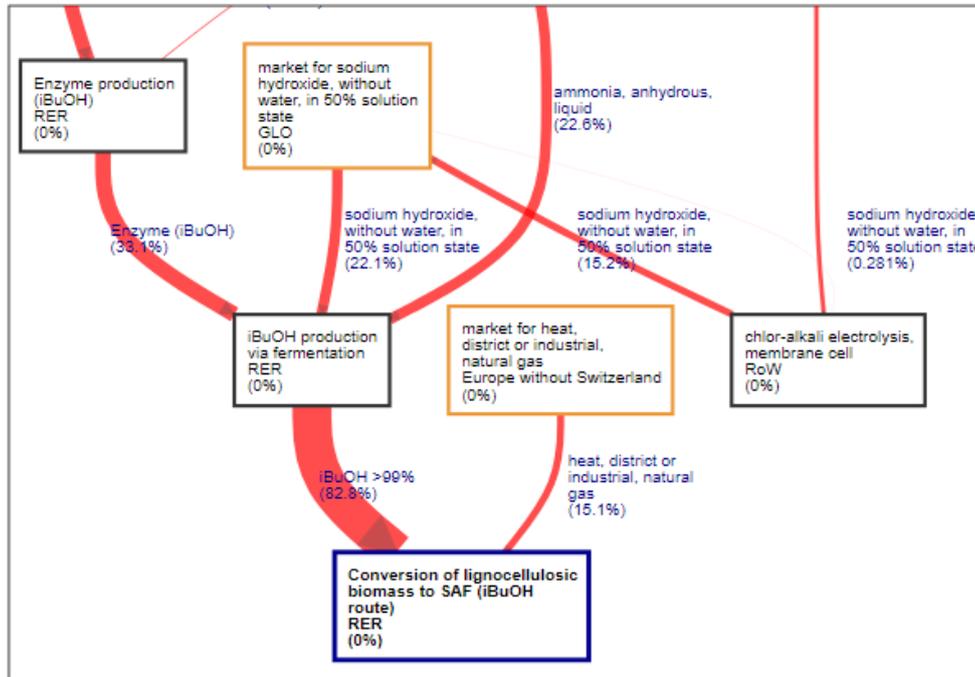
Figure 4.13: Sankey diagram of emissions - EtOH route
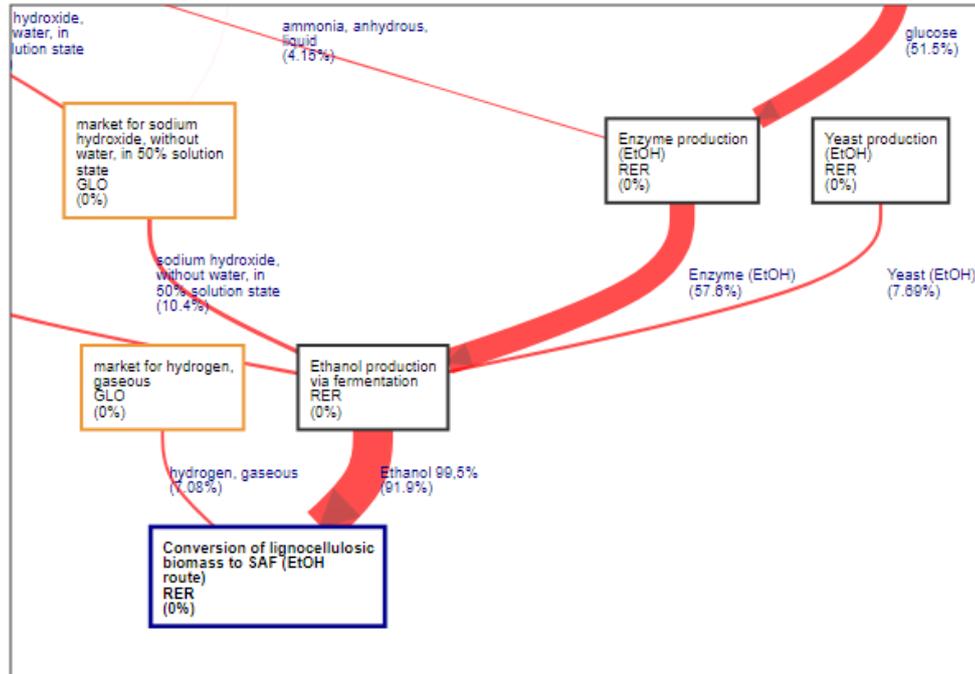
Upon examination of the Isobutene Sankey diagram, depicted in figure 4.13, the following distribution was observed: Sodium hydroxide at 55%, enzyme at 11%, calcium oxide (quicklime) at 9%, sodium chlorate at 9%, and ammonia at 8%. Notably, enzymes account for a smaller share in this case compared to previous instances, while sodium hydroxide and calcium oxide contribute significantly to the overall emissions. This peculiarity can be explained by the role of sodium hydroxide and calcium oxide in the pretreatment of chipped biomass before enzymatic saccharification. Pretreatment is designed to break down the complex lignocellulose structure, enhancing the enzymatic digestibility of the feedstock. A more extensive pretreatment likely results in a reduced need for enzymes in the saccharification process. This underscores how the choice of specifications and technologies for biomass fermentation can lead to variations in inputs and chemical quantities, ultimately influencing emissions based on the selected inventory for a specific production process. The reasons behind the technical decisions driving these variations and their consequences on the process are beyond the scope of this thesis and will not be extensively discussed.

Figure 4.14: Sankey diagram of emissions - IBN route
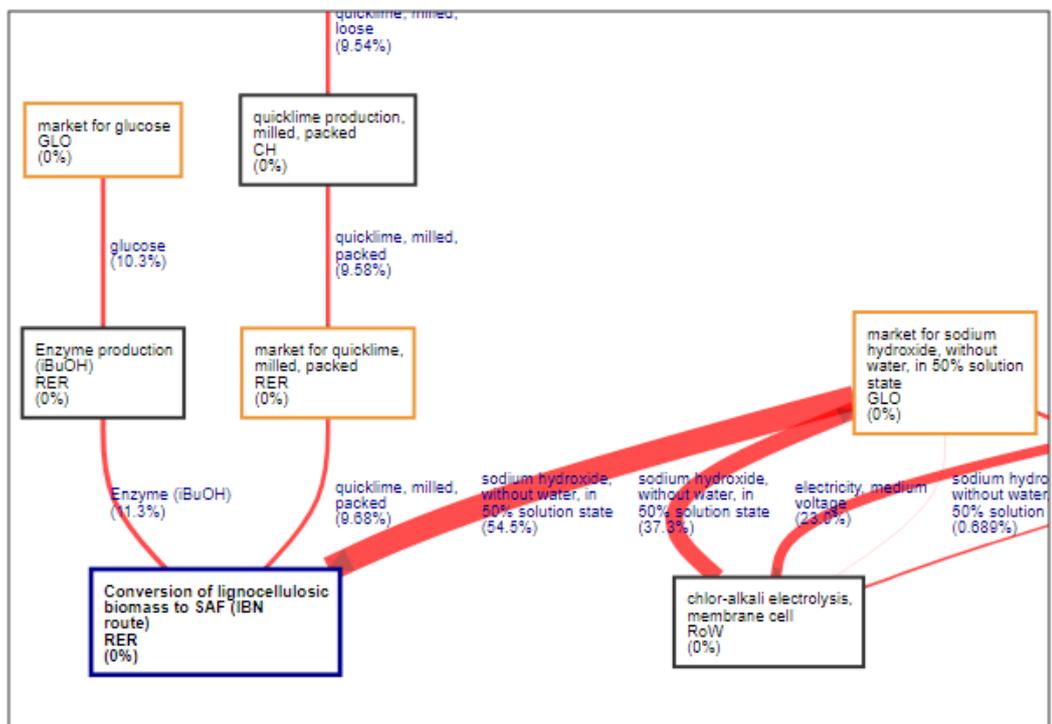
<u>Electricity demand in the different industrial conversion processes</u>

The need of external electricity supply to the industrial process primarily derives from chipping the biomass, running auxiliary systems, and producing enzymes or yeast. The evaluated electricity requirements for the process were determined to be 0.021 kWh MJ_{SAF}^{-1}, 0.0053 kWh MJ_{SAF}^{-1}, and 0.077 kWh MJ_{SAF}^{-1} for the ethanol, isobutanol, and isobutene routes, respectively.

The higher electricity demand for ethanol compared to isobutanol is attributed to the need for electricity to cover the heat process demand and the electricity used to produce the enzyme cellulase. In the enzyme inventory used for isobutanol, electricity was not reported, likely because the amount was considered negligible. Concerning the IBN supply chain, the higher electricity consumption compared to other routes cannot be entirely elucidated due to the sensitive nature of the technology. However, one hypothesis suggests that a portion of this electricity consumption may have been used for on-site hydrogen production. This hypothesis could explain why the hydrogen input in the inventory was lower than expected, although the lower amount is also influenced by the characteristics of the IBN supply chain.

As already mentioned, emission factor significantly varies depending on the public grid mix of the country. These variations emphasize the substantial influence of electricity in differentiating overall emissions among countries. For instance, considering the isobutanol route, emissions associated with electricity consumption vary from 0.10 gCO_2eq MJ_{SAF}^{-1} to 5.15 gCO_2eq MJ_{SAF}^{-1}, with a European average of 2.03 gCO_2eq MJ_{SAF}^{-1}. In contrast, for the IBN route, these values range from 1.47 gCO_2eq MJ_{SAF}^{-1} to 75.33 gCO_2eq MJ_{SAF}^{-1}, with a European average of 29.64 gCO_2eq MJ_{SAF}^{-1}. This underscores how crucial the public grid electricity mix is in determining the suitability of a production route for a specific country.

4.2.4 SAF transportation to airport

While there are disparities among countries in terms of size, the elevated average number of airports, leading to reduced transport distances, and the high energy content of SAF resulting in a low mass per megajoule all contribute to minimal emissions associated with SAF transportation to the biorefinery plant per functional

unit. Emission values vary between 0.34 to 1.01 gCO$_2$eq MJ$_{SAF}^{-1}$, representing less than 2% of the overall life cycle emissions, even considering the worst-case scenario. Data concerning the number of airports, assumed transportation distance and emissions per functional unit can be found in the Appendix.

4.2.5 Feedstock to Jet overall emissions

As noted in the previous sections, the well-to-wings emissions of SAF are influenced by many factors, with results varying by country, route, and feedstock selected. The results for herbaceous energy crops cultivated in abandoned cropland areas are presented in Figures 4.15, 4.16 and 4.17 and are now discussed.

Herbaceous energy crops

Concerning the ethanol route, it is evident across all countries that emissions associated with biomass production constitute a substantial portion of well-to-wings emissions, approximately 20%. As discussed earlier, although this step varies by country, its impact is not the primary factor determining the differences in life cycle emissions among countries. Biomass transport exhibits a wide range of variation and stands out as one of the primary contributors to disparities among nations. For example, in Finland, it accounts for around 22% of overall emissions, while in Lithuania, it represents only approximately 2%. Another significant factor accentuating discrepancies is electricity. Notably, in nations like Norway, Switzerland, or France, with low emissions factors for electricity, electricity consumption contributes around 0.7%, 1.7%, and 3.7%, respectively, to the life cycle emissions. In contrast, in countries such as Estonia or Poland, it contributes around 30% and 32%, respectively. Regarding industrial conversion, the values are assumed to be uniform across all countries, as previously discussed. Transportation of SAF contributes minimally. Thus, considering the ethanol route fed by herbaceous energy crops, overall life cycle emissions range from 42.9 gCO$_2$eq MJ$_{SAF}^{-1}$ for France to 65.3 gCO$_2$eq MJ$_{SAF}^{-1}$ for Finland, with a European average of 52.3 gCO$_2$eq MJ$_{SAF}^{-1}$. Comparing this to a baseline of conventional jet fuel set at

94 gCO$_2$eq MJ$_{SAF}^{-1}$, it implies emissions reduction ranging between 30% and 54% with the use of SAF.

Figure 4.15: Country-based life cycle emissions - SAF ATJ Ethanol route fed by herbaceous crops
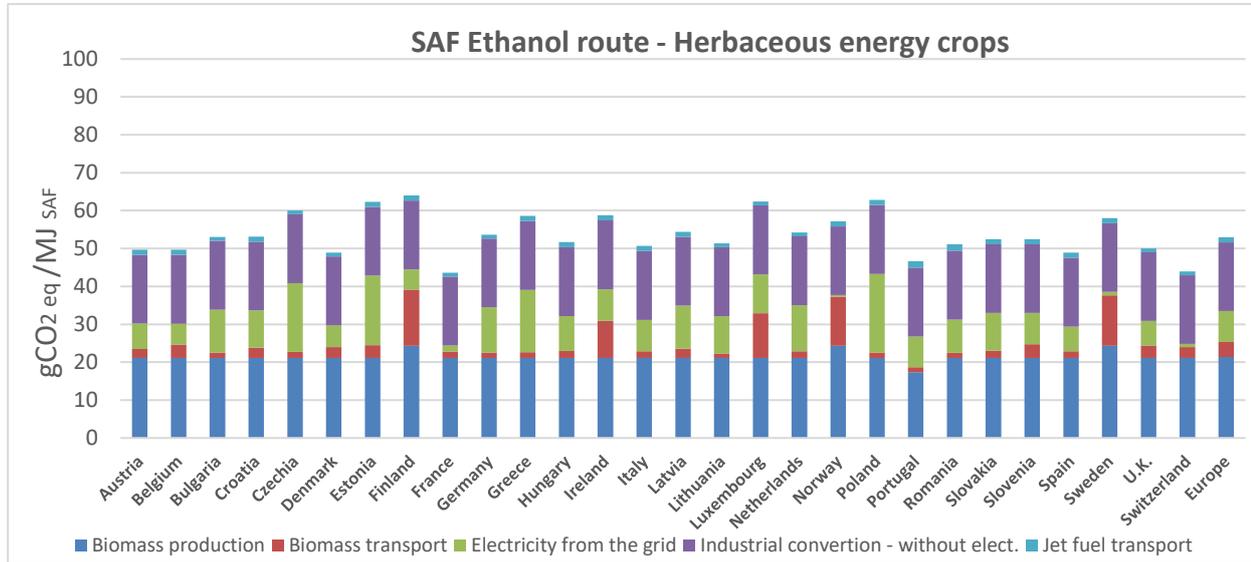
Considering the isobutanol route, similar considerations apply, except for the contribution of electricity demand, which, in this case, is notably lower due to reduced electricity requirements. In this context, well-to-wings emissions range from 41.9 gCO$_2$eq MJ$_{SAF}^{-1}$ for Portugal to 61.7 gCO$_2$eq MJ$_{SAF}^{-1}$ for Finland, with a European average of 48.3 gCO$_2$eq MJ$_{SAF}^{-1}$. This translates to emissions reductions compared to the baseline ranging between 34% and 55%. Portugal's superior performance can be attributed to lower emissions from biomass production, owing to Miscanthus cultivation, and reduced emissions from biomass transport due to the country's high productivity.

Figure 4.16: Country-based life cycle emissions - SAF ATJ Isobutanol route fed by herbaceous crops
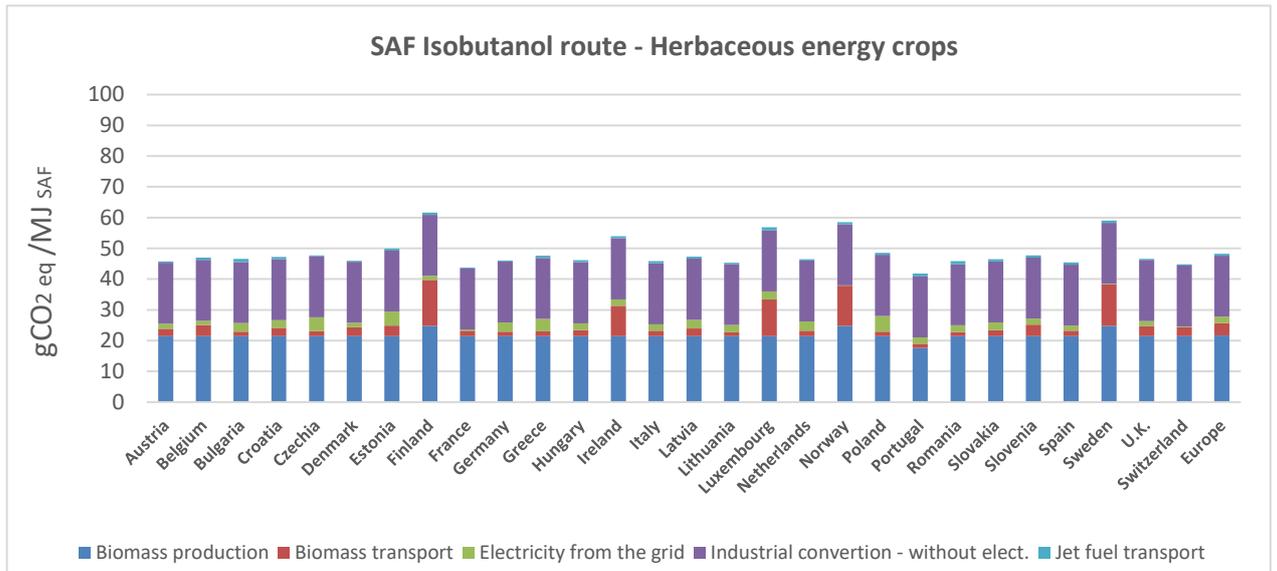
When examining the isobutene route, we immediately observe a significant disparity in the country-based results. This discrepancy arises from the substantial fluctuation in electricity contributions across different countries, attributed to the considerable differences in electricity emissions factors. The well-to-wings emissions range from 37.3 gCO_2eq MJ_{SAF}^{-1} for Switzerland to 108.9 gCO_2eq MJ_{SAF}^{-1} for Poland, with a European average of 65.7 gCO_2eq MJ_{SAF}^{-1}. Excluding the worst-performing countries compared to the baseline, emissions reductions can reach up to 60%.

Figure 4.17: Country-based life cycle emissions – SAF ATJ Isobutene route fed by herbaceous crops
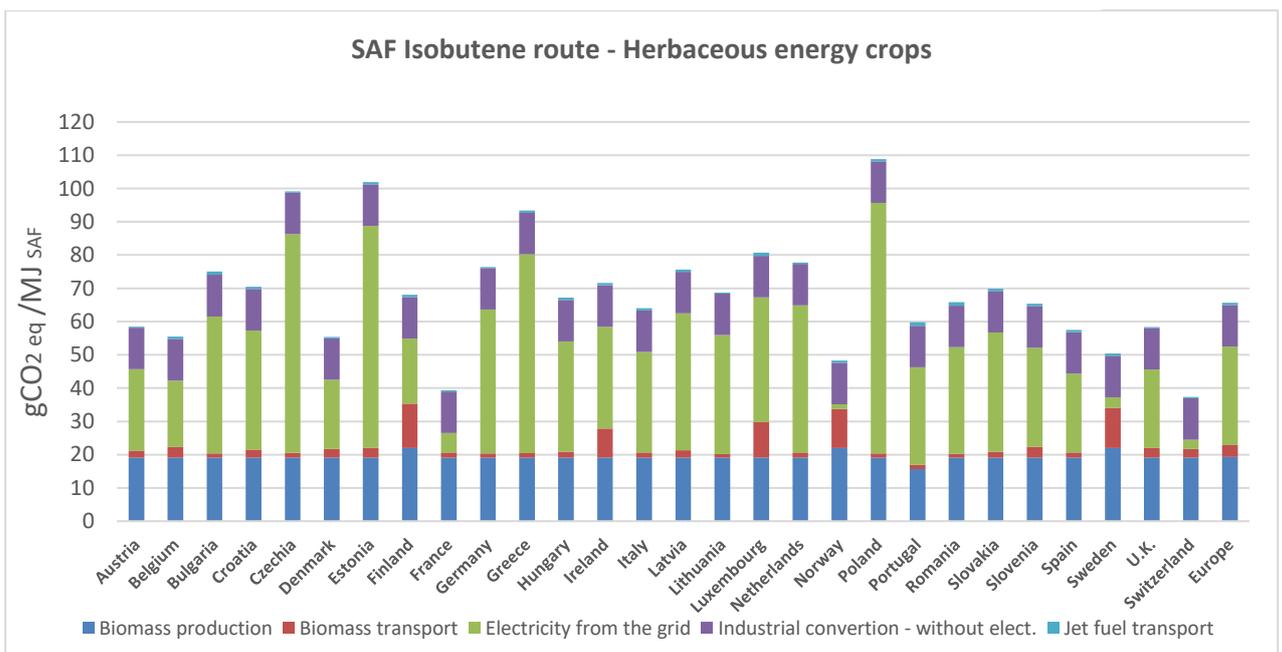
Table 4.4 provides a concise summary of key findings, highlighting the worst and best-performing countries for each route based on emission reduction compared to the baseline. The evaluation indicates that the isobutanol pathway provided best results, leading to a higher average emissions reduction. In contrast, the isobutene route exhibited the least favorable average outcomes, primarily due to the substantial impact of electricity on emissions in many countries. It is worth noting that if we focus solely on countries with a low emission factor for electricity, the isobutene route would emerge as the top-performing option. This is evident in the case of Switzerland, where this route demonstrated the most favorable performance among all pathways, achieving the highest emission reductio, around 60%.

Table 4.4: Summary of emissions performance of different routes – Herbaceous crops

	Ethanol to jet	Isobutanol to jet	Isobutane to jet
	[gCO$_2$/MJ$_{SAF}$]	[gCO$_2$/MJ$_{SAF}$]	[gCO$_2$/MJ$_{SAF}$]
Worst Scenario	63.3 - Finland	61.6 - Finland	108.9 - Poland
Emission reduction	33%	34%	/
Best Scenario	42.9 - France	41.9 - Portugal	37.3 - Switzerland
Emission reduction	54%	55%	60%
Average Europe	52.3	48.3	65.7
Emission reduction	44%	49%	30%

Supplementary scenario

Although in the previous evaluation the isobutanol route demonstrated better performance than the ethanol route, it would be misleading to conclude that it is unequivocally the superior solution due to the small differences in the results and the unaccounted uncertainty in the data. To emphasize this point, another analysis was conducted using only inventories for industrial conversion to SAF provided by the CORSIA Supporting Document, which collected data from various sources and databases in the U.S. context. To simplify the analysis, all inputs were entered into the Brightway2 software without separating the impacts between chemical inputs and electricity inputs as done for the previous scenarios. This means that only the average emission factor for Europe was considered, taken from Ecoinvent 3.9, equal to 350 gCO$_2$ kWh^{-1}.

The simulation results, depicted in Figure 4.18 and 4.19, confirm that there are no significant differences between the two pathways in terms of well-to-wings emissions. Furthermore, the graphs highlight once again the larger emission gap occurring during the conversion from EtOH to SAF compared to the gap in the conversion from i-BuOH to SAF, whose reasons were previously discussed in the preceding paragraphs. Still, the isobutene pathway exhibits higher average emissions due to higher electricity demand.

Figure 4.18: Emissions concerning alcohols production process with electricity for different route – Supp. scenario
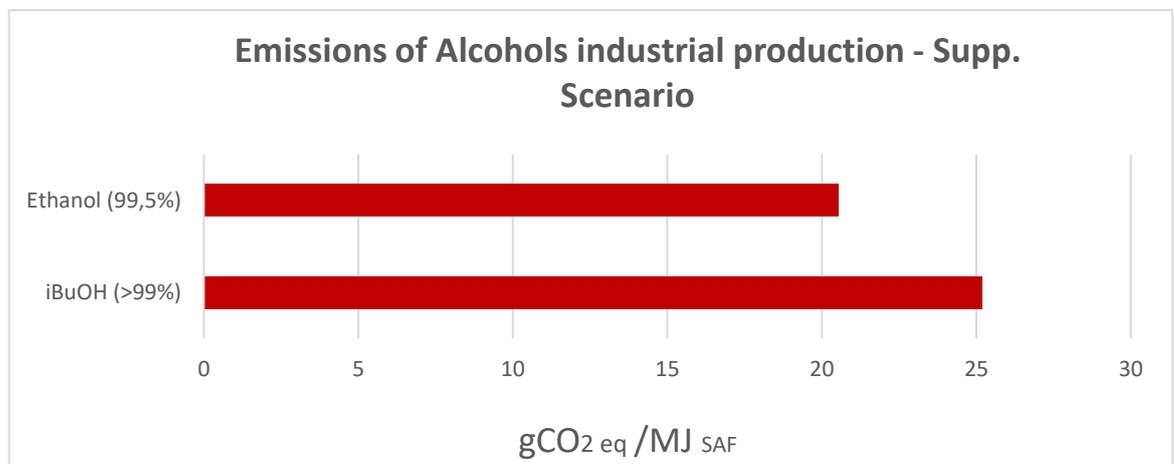
Figure 4.19: Emissions concerning SAF conversion process with electricity for different route – Supp. scenario
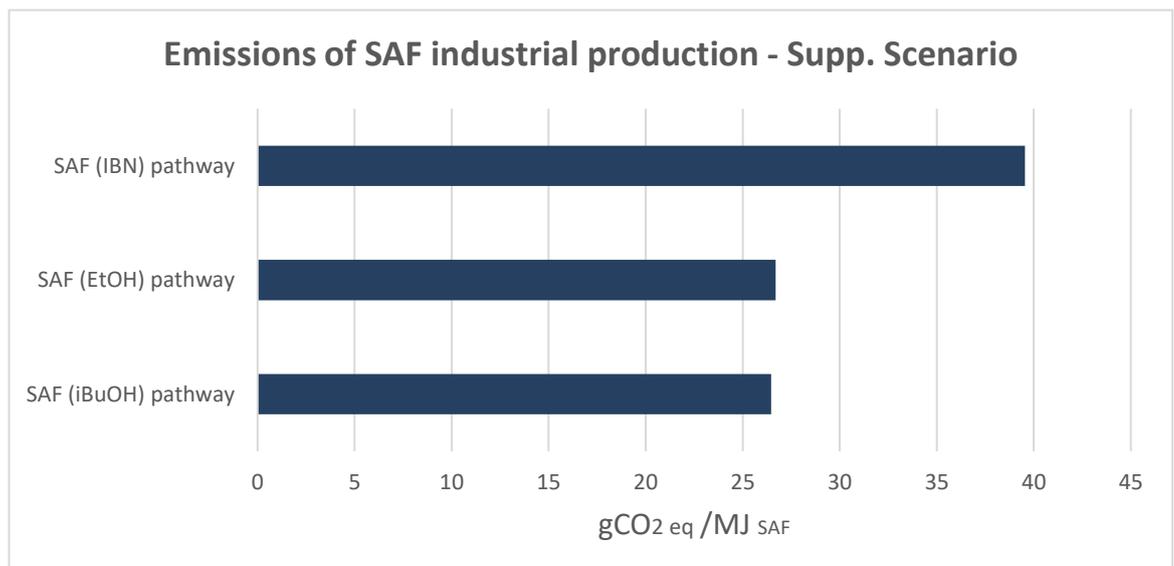
Agricultural and forestry residues

The discussion now turns to the presentation of results for sustainable aviation fuel supply chains (SAFs) in agriculture and forestry, represented visually in Figures 4.20, 4.21, and 4.22. Most of the main results are in line with those of the previous scenarios, which leads us to focus only on the distinctive results.

Starting from the ethanol pathway, it is clear that the impact of transport-related emissions (biomass transport and SAF transport) on overall well-to-wings emissions is almost negligible. The predominant contributions come from electricity and chemicals used in industrial conversion processes. Excluding emissions from biomass production, which contribute about 20 gCO_2eq MJ_{SAF}^{-1} in scenarios using herbaceous energy crops, country-specific emissions show a significant decrease from previous assessments. The results range from 20.7 to 40.6 gCO_2eq MJ_{SAF}^{-1} in Switzerland and Poland, respectively, with a European average of 28.2 gCO_2eq MJ_{SAF}^{-1}. This implies a significant reduction in emissions, ranging from 56% to 78% compared to the reference scenario.

Figure 4.20: Country-based life cycle emissions – SAF ATJ Ethanol route fed by residues
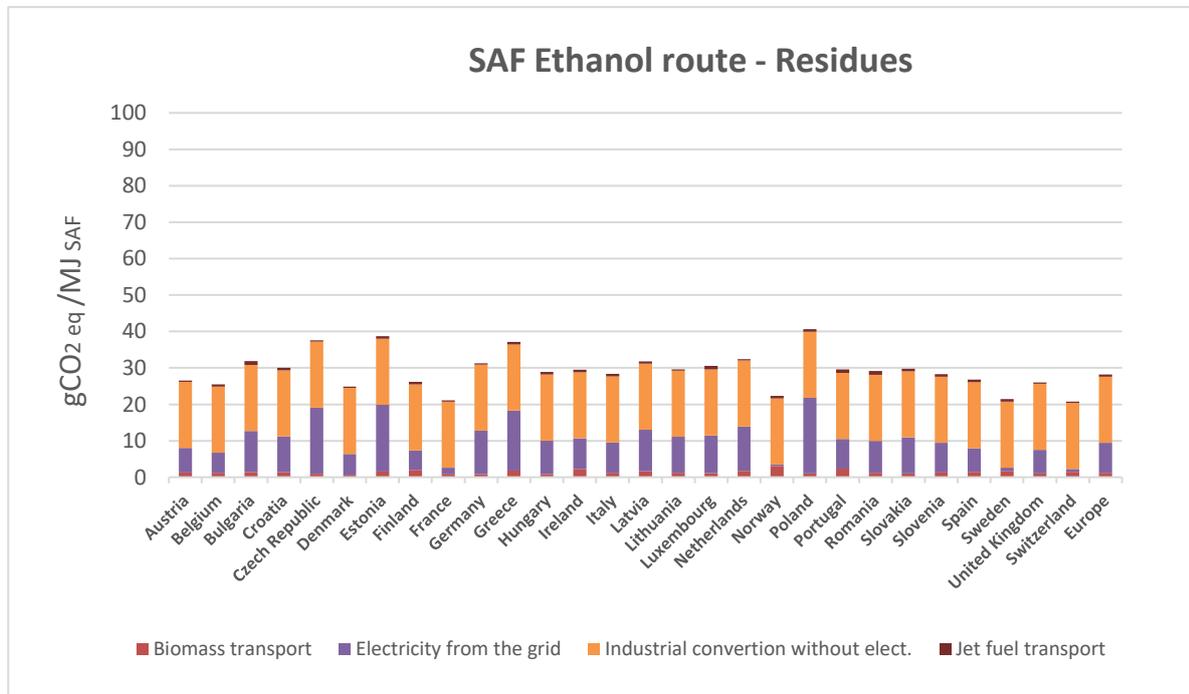
Similar trends are observed in the ATJ via i-BuOH route, with the notable exception that the contribution of electricity is noticeably reduced compared to EtOH in shaping the overall emissions. The results range from 21.6 gCO_2eq MJ_{SAF}^{-1} in France to 26.8 gCO_2eq MJ_{SAF}^{-1} in Poland, with a European average of 23.8 gCO_2eq MJ_{SAF}^{-1} This signifies a significant reduction in emissions compared to the baseline associated with fossil kerosene, ranging between 71% and 78%.

Figure 4.21: Country-based life cycle emissions - SAF ATJ Isobutanol route fed by residues
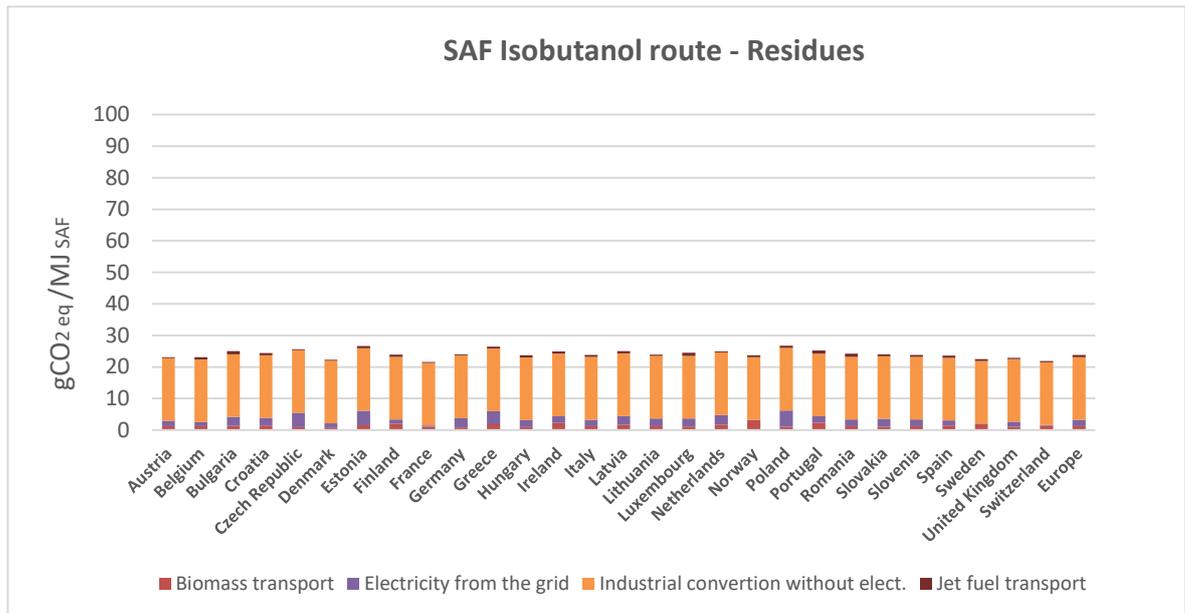
In the scenario involving the isobutene supply chain, there are observable fluctuations in the results. Emissions display a considerable range, extending from 16.9 gCO_2eq MJ_{SAF}^{-1} for Switzerland to 89.4 gCO_2eq MJ_{SAF}^{-1} for Poland, with an average of 43.9 gCO_2eq MJ_{SAF}^{-1}. This implies dramatic varying degrees of emissions reductions compared to the baseline associated with fossil kerosene, spanning from 5% to 82%.

Figure 4.22: Country-based life cycle emissions - SAF ATJ Isobutene route fed by residues

SAF Isobutene route - residues

Legend: ■ Biomass transport ■ Electricity from the grid ■ Industrial convertion without elect. ■ Jet fuel transport
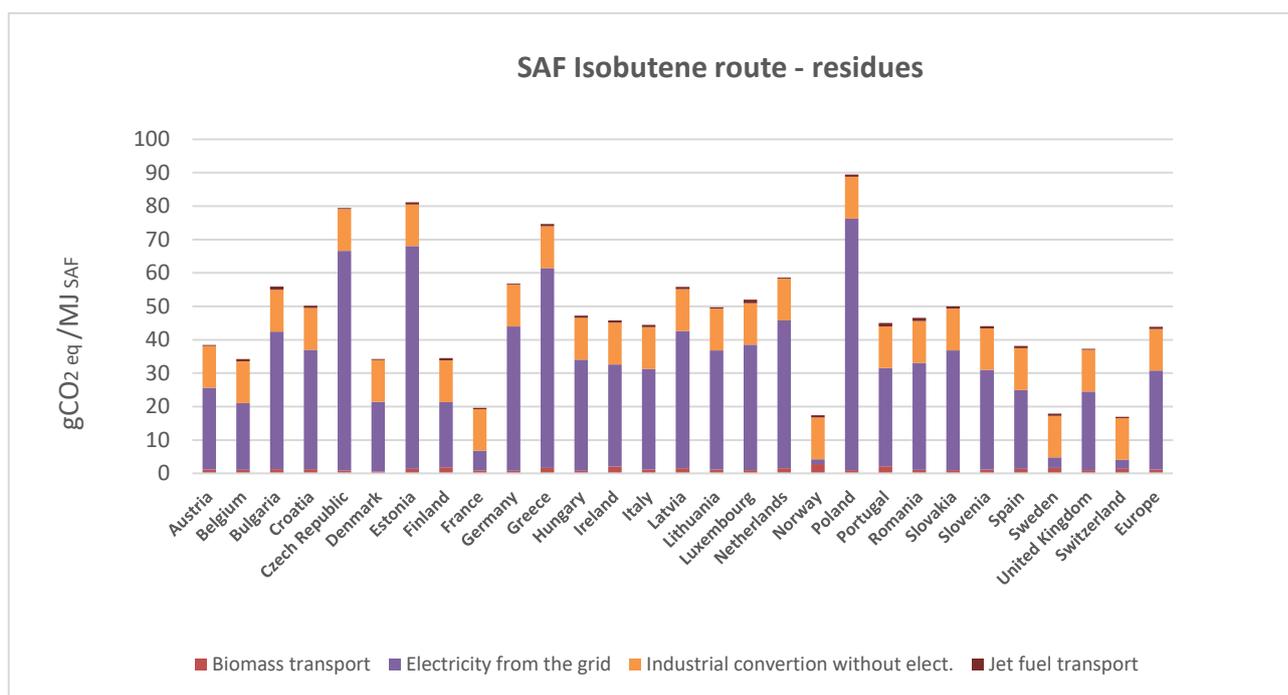
In Table 4.8, a concise overview of key results highlights the best and worst performing countries for each pathway based on emission reduction. Notably, isobutene shows the lowest emissions for a specific country, while the isobutanol pathway shows a higher average emission reduction. Interestingly, the optimal scenario for the ethanol pathway outperforms that of the isobutanol pathway, emphasizing comparable emissions within the supply chains. Variability in the results is strictly influenced by inventory selection, which may tip the balance toward either pathway.

Table 4.5: Summary of emissions performance of different routes – Residues crops

	Ethanol to jet	Isobutanol to jet	Isobutane to jet
	[gCO2/MJSAF]	[gCO2/MJSAF]	[gCO2/MJSAF]
Worst Scenario	40.6 - Poland	26.8 - Poland	89.4 - Poland
Emission reduction	56%	71%	5%
Best Scenario	20.7 - Switzerland	21.6 - France	16.9 - Switzerland
Emission reduction	78%	78%	82%
Average Europe	282	23,8	43,9
Emission reduction	70%	75%	53%

4.3 Scale-up potential to meet the forecasted aviation fuel demand

Based on the 2019 data on country-specific jet fuel demand [87], the projected aviation fuel demand for 2025 was determined, assuming a fully recovering from the pre-pandemic COVID-19 levels as suggested by IEA [4]. The estimated total jet fuel demand in the European countries selected in this analysis is 488.8 Million barrels per year (Mbpy), with UK, Germany and France leading with 97.1, 80.7, 62.4, and 36.2 Mbpy, respectively. Without efforts toward a more sustainable aviation industry, this fuel consumption would result in estimated emissions of around 263.9 Mton CO_2eq year^{-1}, according to the baseline of 94 gCO_2eq MJ^{-1} set by the directive EU RED 2018/2001/EC Annex V C 19.

To gauge the potential of SAF production through ATJ pathways from lignocellulosic feedstock, optimal scenarios were explored for each country. These scenarios aimed to maximize SAF production with the lowest emissions and the best savings compared to the baseline. At European level, the available feedstock exploitable for this purpose was estimated to be approximately 98 million tons of dry biomass per year (Mton$_{db}$ year^{-1}) for herbaceous energy crops in abandoned cropland areas and around 160 Mton$_{db}$ year^{-1} for agricultural and forestry residues. In this hypothetical exercise to estimate the potential of SAF production in Europe, we consider assumed that all available agricultural and forestry residues would be prioritized to the production of SAF via ATJ route. If production fell short of covering the country's jet fuel demand, herbaceous energy crops cultivated in abandoned cropland area would be tapped into. This strategic decision was based on earlier findings indicating significantly lower emissions per functional unit from SAF production using residues compared to grass exploitation. Also, residues are widely accepted as a sustainable feedstock source for the production of advanced biofuels according to RED II.

Another crucial factor is the selection of the ATJ best pathway for each country, influenced by specific emissions per functional unit and the potential SAF yield per unit of reference biomass in input. The i-BuOH pathway was deemed optimal for all European countries, despite other pathways occasionally presenting lower life cycle emissions per megajoule of SAF produced. In fact, the real yield of SAF,

when considering the influence of co-products, significantly contributes to diminish the potential SAF production from EtOH and IBN pathways. With reference to 100 kg of input biomass, the yield in terms of kg of SAF, correspond to 2.8 kg, 2.13 kg, and 1.41 kg per isobutanol, ethanol and isobutene respectively. The production of SAF via the three different routes involves various final by-products and co-products. Although this thesis did not extensively explore the production and potential utilization of these by-products and co-products, it acknowledges their value in supply chains beyond aviation. Consequently, the i-BuOH pathway, known for its selectivity in SAF production, stands out as the most suitable pathway for all countries.

The total potential SAF production at European level was estimated at around 287.1 Mbpy, comprising 178 Mbpy from total residue exploitation and 109.1 Mbpy from total herbaceous energy crops exploitation which could potentially be cultivated in abandoned cropland areas. Considering that, there is a potential to cover approximately 60% of current European jet fuel demand, on average. However, due to disparities in resource availability among countries, these potentials can be either higher or lower depending on the country. For instance, examining the local potential of ATJ production reveals that some countries like Romania or Slovakia, exhibit the potential to cover over 10 times their jet fuel demand due to higher biomass availability and relatively lower fuel demand; on the other hand, the opposite scenario is observed in Luxemburg or the Netherlands, whose potential ATJ-based SAF production would supply only a small percentage of the demand (2.6% and 5.6%, respectively).

Initially, the study explored a trade scenario involving the exchange of biomass resources among countries to address shortages in specific regions, simplifying by neglecting transport emissions associated with the trades. The primary goal was to fully exploit lignocellulosic resources and evaluate the climate change mitigation possibilities arising from their comprehensive utilization.

The detailed results in Table 4.9 include the potential ATJ SAF production for each country and the respective SAF percentage covering country-specific jet fuel demand. The subsequent column outlines the additional conventional jet fuel

needed to cover the country-specific SAF shortage. Negative values in some countries, where ATJ SAF production exceeds demand, partially offset these requirements through trades. Overall, the additional kerosene fuel required to meet the remaining demand not covered by SAF, approximately 40% of European jet fuel demand, amounts to 201.6 Mbpy. Divergent feedstock availability among countries results in notable fluctuations in climate change mitigation potential, spanning from 1.9% in Luxembourg to 902.1% in Romania, as shown in Figure 4.22. The results indicate a potential emission saving of 102.5 million tons of CO_2eq and a climate change mitigation potential of 38.8% at the European level compared to the baseline scenario that was assessed by multiplying country-specific jet fuel demand values to the baseline of 94 gCO_2eq MJ^{-1}.

Table 4.6: Country-based potential emission saving per year in Europe – trading scenario

Country	Jet fuel demand in 2025	Potential of ATJ-based SAF production	% of SAF supply to meet the fossil jet fuel demand	Additional kerosene to cover the shortage	Estimated emission by exploiting SAF	Estimated emission in baseline scenario	Share respect to baseline	Emission savings	Climate change mitigation potential share
	Mbpy	Mbpy	%	Mbpy	Mton CO_2 yr	Mton CO_2 yr	%	Mton CO_2 yr	%
Austria	7.7	4.3	55.5%	3.4	2.6	4.1	62.2%	1.6	37.8%
Belgium	13.5	1.4	10.6%	12.1	6.7	7.3	92.4%	0.6	7.6%
Bulgaria	1.9	8.3	447.2%	-6.5	-1.7	1.0	-167.9%	2.7	267.9%
Croatia	1.6	2.4	150.4%	-0.8	0.0	0.8	-1.4%	0.9	101.4%
Czechia	3.5	7.3	207.4%	-3.8	-0.6	1.9	-33.5%	2.6	133.5%
Denmark	8.0	5.5	67.9%	2.6	2.1	4.3	49.5%	2.2	50.5%
Estonia	0.5	1.4	252.7%	-0.8	-0.2	0.3	-66.0%	0.5	166.0%
Finland	7.3	4.6	63.0%	2.7	2.1	3.9	53.7%	1.8	46.3%
France	62.4	48.8	78.2%	13.6	15.0	33.7	44.6%	18.7	55.4%
Germany	80.7	42.2	52.4%	38.4	28.4	43.5	65.2%	15.1	34.8%
Greece	11.3	7.3	64.7%	4.0	3.9	6.1	63.6%	2.2	36.4%
Hungary	2.2	9.1	413.6%	-6.9	-2.2	1.2	-185.3%	3.4	285.3%
Ireland	8.4	0.8	10.1%	7.5	4.2	4.5	92.8%	0.3	7.2%
Italy	38.0	19.8	52.1%	18.2	13.6	20.5	66.3%	6.9	33.7%
Latvia	1.2	2.2	180.4%	-1.0	-0.1	0.7	-15.1%	0.7	115.1%
Lithuania	1.0	6.3	615.8%	-5.3	-1.5	0.6	-272.0%	2.1	372.0%
Luxembourg	4.7	0.1	2.6%	4.6	2.5	2.6	98.1%	0.0	1.9%
Netherlands	30.3	1.7	5.6%	28.6	15.8	16.4	96.7%	0.5	3.3%
Norway	7.3	2.4	32.9%	4.9	3.0	3.9	75.2%	1.0	24.8%
Poland	8.4	29.1	346.9%	-20.7	-5.0	4.5	-111.1%	9.6	211.1%
Portugal	12.8	5.0	39.3%	7.8	5.3	6.9	76.9%	1.6	23.1%
Romania	1.5	21.3	1462.0%	-19.9	-6.3	0.8	-802.1%	7.1	902.1%

Slovakia	0.3	3.6	1086.3%	-3.2	-1.1	0.2	-630.9%	1.3	730.9%
Slovenia	0.2	0.8	386.8%	-0.6	-0.2	0.1	-173.9%	0.3	273.9%
Spain	54.4	27.5	50.6%	26.9	19.9	29.4	67.9%	9.4	32.1%
Sweden	8.0	7.8	97.0%	0.2	1.2	4.3	27.0%	3.2	73.0%
U.K.	97.1	14.6	15.0%	82.5	46.7	52.4	89.1%	5.7	10.9%
Switzerland	14.6	1.4	9.9%	13.2	7.3	7.9	92.8%	0.6	7.2%
Europe	488.8	287.2	58.7%	201.6	161.4	263.9	61.2%	102.5	38.8%

*Figure 4.23: Country-based climate change mitigation potential share compared to the baseline -
trading scenario*
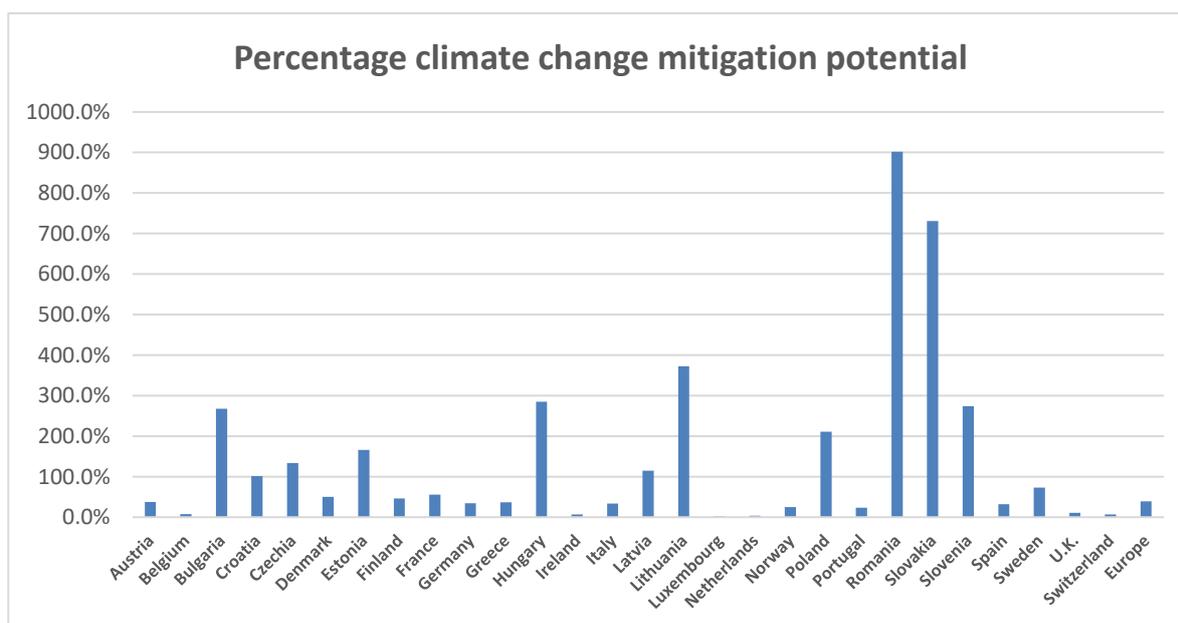
Due to the oversimplification referred to the trade-scenario, the consideration was also given to a non-trade scenario, where the trading of biomass resources among countries was excluded. Instead, these resources could only be exploited within the borders of the country where they were originally produced.

The potential SAF production with full use of all country-based residues and closing the gap of fuel demand with exploitation of Herbaceous crops is estimated equal to 217.7 Mbpy of SAF which could cover around 45% of European jet fuel demand. In such context, the emissions saving might reach up to 80.2 Mton CO_2eq per year, equivalent to 30.4% of emissions released in the baseline scenario. The climate change mitigation potential share ranges from 1.9% in Luxemburg to 74.8% in Hungary. As can be visualized in Figure 4.23. Luxembourg's underperformance is attributed to the scarcity of available lignocellulosic feedstock, preventing the production of the total jet fuel demand. In contrast, Hungary's high performance is

credited to the large availability of residues, which can cover the entirety of the jet fuel demand. Additional information according to assumption and calculations are reported in the Appendix, while country-based results are presented in table 4.10.

Table 4.7: Country-based potential emission saving per year in Europe – not-trading scenario

Country	Current Jet fuel demand	Potential of ATJ-based SAF production *	% of SAF supply to meet the jet fuel demand	SAF production to cover fuel demand	Estimated emission by exploiting SAF **	Estimated emission in baseline scenario	Share respect to baseline	Emission savings	Climate change mitigation potential share
	Mbpy	Mbpy	%	Mbpy	Mton CO$_2$ yr	Mton CO$_2$ yr	%	Mton CO$_2$ yr	%
Austria	7.7	4.3	55.5%	4.3	2.6	4.1	62.2%	1.6	37.8%
Belgium	13.5	1.4	10.6%	1.4	6.7	7.3	92.4%	0.6	7.6%
Bulgaria	1.9	8.3	447.2%	1.9	0.3	1.0	26.6%	0.7	73.4%
Croatia	1.6	2.4	150.4%	1.6	0.2	0.8	25.9%	0.6	74.1%
Czechia	3.5	7.3	207.4%	3.5	0.5	1.9	27.3%	1.4	72.7%
Denmark	8.0	5.5	67.9%	5.5	2.1	4.3	49.5%	2.2	50.5%
Estonia	0.5	1.4	252.7%	0.5	0.1	0.3	28.3%	0.2	71.7%
Finland	7.3	4.6	63.0%	4.6	2.1	3.9	53.7%	1.8	46.3%
France	62.4	48.8	78.2%	48.8	15.0	33.7	44.6%	18.7	55.4%
Germany	80.7	42.2	52.4%	42.2	28.4	43.5	65.2%	15.1	34.8%
Greece	11.3	7.3	64.7%	7.3	3.9	6.1	63.6%	2.2	36.4%
Hungary	2.2	9.1	413.6%	2.2	0.3	1.2	25.2%	0.9	74.8%
Ireland	8.4	0.8	10.1%	0.8	4.2	4.5	92.8%	0.3	7.2%
Italy	38.0	19.8	52.1%	19.8	13.6	20.5	66.3%	6.9	33.7%
Latvia	1.2	2.2	180.4%	1.2	0.2	0.7	26.6%	0.5	73.4%
Lithuania	1.0	6.3	615.8%	1.0	0.1	0.6	25.4%	0.4	74.6%
Luxembourg	4.7	0.1	2.6%	0.1	2.5	2.6	98.1%	0.0	1.9%
Netherlands	30.3	1.7	5.6%	1.7	15.8	16.4	96.7%	0.5	3.3%
Norway	7.3	2.4	32.9%	2.4	3.0	3.9	75.2%	1.0	24.8%
Poland	8.4	29.1	346.9%	8.4	1.3	4.5	28.5%	3.2	71.5%
Portugal	12.8	5.0	39.3%	5.0	5.3	6.9	76.9%	1.6	23.1%
Romania	1.5	21.3	1462.0%	1.5	0.2	0.8	25.8%	0.6	74.2%
Slovakia	0.3	3.6	1086.3%	0.3	0.0	0.2	25.6%	0.1	74.4%
Slovenia	0.2	0.8	386.8%	0.2	0.0	0.1	25.4%	0.1	74.6%
Spain	54.4	27.5	50.6%	27.5	19.9	29.4	67.9%	9.4	32.1%
Sweden	8.0	7.8	97.0%	7.8	1.2	4.3	27.0%	3.2	73.0%
U.K.	97.1	14.6	15.0%	14.6	46.7	52.4	89.1%	5.7	10.9%
Switzerland	14.6	1.4	9.9%	1.4	7.3	7.9	92.8%	0.6	7.2%
Europe	488.8	287.2	58.7%	217.7	183.7	263.9	69.6%	80.2	30.4%

*Potential ATJ-based SAF considering the full exploitation of herbaceous crops and residues

** Emissions including the use of SAF from crops and herbaceous residues and additional fossil jet fuel offset in case of insufficient SAF production

Climate change mitigation potential
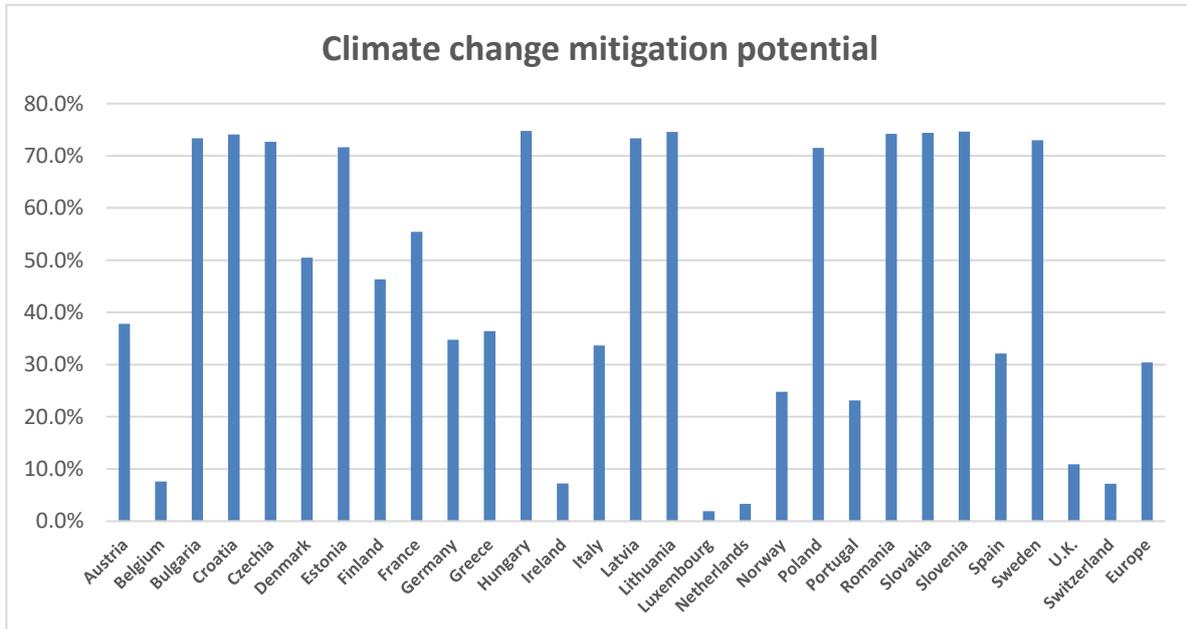
Conclusion

<u>Limitation of the study</u>

This research provides valuable insights to the ongoing efforts to enhance the sustainability of aviation fuels, offering a foundation for future studies and advancements in the field. However, several limitations were addressed to the study due to the unavailability of data and assumptions that constrain the reliability of the results and stimulate new research and refinements.

The study's analysis utilized chosen inventories from the literature to formulate supply chains for different pathways. Despite a justified selection process, the results are influenced by the authors' technical choices and specifications, potentially leading to varied outcomes, as demonstrated in supplementary scenarios using CORSIA inventories. Moreover, the progression of technology and the commercial scaling of SAF production pathways may lead to more efficient integrated facilities, capable of reducing overall consumption and achieving better energy efficiency of the production processes. The study also underscores the importance of considering the broader impact and valuability of by-products and co-products in achieving a holistic assessment of SAF production pathways.

The isobutene route, while promising for high selectivity in the production of SAF, faces obstacles such as limited documentation and lower TRL than the i-BuOH and EtOH routes. These factors introduce uncertainties in the available data and complete understanding of the isobutene production process. Addressing these challenges requires further research and development efforts to enhance reliability and propel the isobutene pathway to a higher level of maturity in SAF production.

Furthermore, it is crucial to acknowledge the optimistic assumption underpinning the thesis's scenarios: the possibility of fully exploiting all available residues and energy crops in abandoned cropland areas. Recognizing the value of these raw materials in other industries and considering the emissions within its SAF supply chain are essential factors. Fully utilizing abandoned cropland areas for herbaceous energy crops may present challenges and their exploitation may not be justifiable by their limited climate change mitigation potential.

Finally, this thesis utilizes a uniform feedstock source for all supply chains, overlooking diverse biomass compositions and potentially impacting outcomes such as yield, carbon, and energy efficiencies.

<u>Closing remarks</u>

The aim of this thesis was assessing the environmental impacts of sustainable jet fuels produced from lignocellulosic biomasses through the alcohol-to-jet pathway, incorporating ethanol and isobutanol as approved feedstocks and exploring isobutene as a potential future intermediate.

Comparative assessments between ethanol and isobutanol routes reveal several differences in their yield performance when considering the overall supply chain: whereas EtOH stands out for its higher mass yield of chemical intermediates respect to i-BuOH (27% vs 19%) the latter showed better yields performance in the subsequent conversion step to produce SAF (74% vs 42%). This highlights the higher selectivity of i-BuOH route to produce SAF instead of other biofuel co-products, revealed also by the Carbon and Energy efficiencies analysis.

The study extends its evaluation to the Isobutene pathway, which emerges as a promising option for inclusion in aviation fuel standards. Despite limited information on the production process, the Isobutene pathway manifests the highest conversion efficiency, as evidenced by the lowest feedstock demand, in transforming lignocellulosic biomass into SAF when considering energy allocation. Its advantageous absence of co-produced fuels highlights its high selectivity for SAF production, with an evaluated feedstock demand per functional unit of 0.117 kg_{db} MJ_{SAF}^{-1} compared to 0.130 kg_{db} MJ_{SAF}^{-1} and 0.132 kg_{db} MJ_{SAF}^{-1} for ethanol and isobutanol, respectively. However, the Isobutene route exhibits the lowest carbon efficiency (23.9%) due to a lower IBN yield, attributed to reduced exploitation of sugars in the feedstock, resulting in higher carbon delivered to by-products like lignin or C5 sugars. The Isobutene supply chain stands out for its superior energy efficiency (47.5%), despite a high electricity requirement, enhanced by the high energy value of by-products such as lignin, ethanol, sludge, and microbial biomass across various industries, and lower hydrogen demand in the industrial process.

The findings emphasize the overall superiority of i-BuOH and IBN pathway in enhancing SAF production compared to other fuel co-products. However, it is worth noting that additional scrutiny and comprehensive studies are necessary to validate these findings, despite their alignment with previously reported literature. Additionally, EtOH pathway still maintains a superior yield of the intermediate alcohol, a milestone that the i-BuOH pathway is yet to achieve despite its advanced TRL. Advancements in technologies, such as new engineering yeasts are necessary to boost to isobutanol and isobutene yield and enhance SAF production.

The life cycle assessment of environmental impacts, particularly GHG intensities, sheds light on the variations occurring among country, route, and selected feedstock.

Referring to the routes involving herbaceous energy crops, biomass production and industrial conversion emissions constituted a significant portion of well-to-wings emissions across all countries. Key contributors to emission variations among nations included biomass transport and electricity.

Shifting to supply chains involving agricultural and forestry residues, transport-related emissions had a negligible impact on overall well-to-wings emissions for both ethanol, isobutanol and isobutene routes. Predominant contributions came from electricity and chemicals used in industrial conversion processes.

The isobutanol pathway consistently provided better results, with higher average emissions reduction. In contrast, the isobutene route showed less favorable outcomes, primarily due to the substantial impact of electricity on emissions in many countries. However, focusing on countries with low electricity emission factors could make the isobutene route the top-performing option, as observed in Switzerland and France.

The study also addresses the scale-up potential of SAF production to meet current aviation fuel demand. Optimal scenarios were explored for each European country, aiming to maximize SAF production with minimal emissions. The i-BuOH pathway emerged as the most suitable option for all countries, considering specific emissions and potential SAF yield. This highlights an important consideration regarding

pathways with favorable GWP but low SAF yield: a low SAF yield, attributed to various factors we have explored, has the potential to hinder the scalability of routes with low GWP. In contrast, it tends to favor routes with higher GWP, as long as they can generate more SAF per unit of biomass input. This, in turn, enables a more effective substitution of fossil kerosene, resulting in reduced overall emissions. Nevertheless, this consideration does not incorporate the possible utilization of by- and co-products generated in the value chain, such as lignin, ethanol, sludge, and microbial biomass. These resources are valuable and could potentially contribute to emissions reduction in other supply chains, however, the primary focus of this study was on SAF production rather than an assessment of the by- and co-products.

The total potential SAF production, incorporating both herbaceous energy crops and agricultural/forestry residue utilization, could meet approximately 60% of the current European jet fuel demand in a trade scenario. The total emissions, considering both SAF usage and additional kerosene fuel for the remaining 40% of demand, were estimated at 61% of baseline scenario emissions, indicating a climate potential mitigation share of 39%. However, country-specific disparities highlight the necessity for tailored strategies. In a non-trade scenario, there would be the potential to cover about 45% of European jet fuel demand results in a climate potential mitigation share of around 30%.

Certainly, the scale-up analysis is not intended to mirror the projections of the European Space Agency, which forecasts that SAF ATJ will contribute about 20% of total SAF supply in Europe by 2050, which in turn will cover about 70% of total jet fuel demand. This underscores the critical need to investigate and incorporate various feedstocks, production pathways, and technologies like HEFA, Power to Liquid and Gasification+FT to push SAF production and achieve complete coverage of jet fuel demand in the coming decades.

In light of these consideration, future works should be assessed to better achieve a comprehensive understanding of the processes and to refine the results achieved in this elaborate. The goal is to consider the complex interplay of factors influencing resource availability, future technological advances, commercial-scale deployment

of pathways, and potential climate change mitigation resulting from the introduction of SAF to enable a new, more sustainable aviation industry to take off.

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Appendix

6.1 Biomass production

Concerning the herbaceous energy crops cultivations (bioenergy crops cultivated in abandoned cropland areas), basing on the study of Gvein et al. [79], Switchgrass demonstrates the highest suitability for the agroclimatic conditions in European countries, emerging as the most favorable option for 24 out of 28 countries. In contrast, Reed Canary exhibits compatibility with Norway and Finland, and Miscanthus is the best choice only for Portugal. On the other hand, when considering emissions associated with biomass production, Miscanthus proves to be the most favorable, with approximately 133 gCO_2eq kg_{db}^{-1}. In comparison, Switchgrass and Reed Canary show emissions of 162.9 gCO_2eq kg_{db}^{-1} and 187.6 gCO_2eq kg_{db}^{-1}. The emissions related to biomass production per functional unit were been evaluated by multiplying the emissions related to the production of 1 kg of dry-basis biomass to the feedstock demand to produce 1 MJ of SAF, specific for each route. As shown in the example below.

i.e. Austria (EtOH route) : $$162.9 \frac{gCO_2}{kg_{db}} \cdot 0.1298 \frac{kg_{db}}{MJ_{SAF}} = 21.15 \frac{gCO_2}{MJ_{SAF}}$$

6.2 Biomass transportation to Biorefinery facilities

Biomass transport emissions exhibit variability based on the availability of herbaceous crops and agroforestry residues in different European countries, considering optimal distances from fields to biofuel plants with a capacity of 560 $kton_{db}$ $year^{-1}$. According to study from Watanabe et al. [51], in the context of herbaceous energy crops, transport-related emissions per kilogram of dry biomass range from a minimum of 9 gCO_2eq kg_{db}^{-1} in Lithuania to a maximum of 113.6 gCO_2eq kg_{db}^{-1} in Finland, with the average European value at 30.5 gCO_2eq kg_{db}^{-1}, as reported in the following table.

Lithuania's comparatively lower emissions can be attributed to its highest ratio between potential herbaceous energy crop production and the country's area among European nations. With an average annual European value of around 20 ton_{db} km^2year^{-1}, Lithuania demonstrates a capacity of approximately 54 ton_{db} km^2year^{-1}.

This elevated potential results from the widespread cultivation of herbaceous energy crops on marginal land in Lithuania, leading to reduced distances to various biorefining plants. Conversely, Finland, possessing one of the largest land areas in Europe and a potential production around 3% of the European average, resulting in a ratio of 0.33 ton_{db} $\text{km}^2\text{year}^{-1}$, exhibits the highest emissions associated with biomass transportation. The next figure provides an illustration of the Potential production-country area ratio for all European countries.

Regarding agroforestry residues, similar considerations apply. As depicted in Figure, Denmark exhibits the highest specific potential production at 105 ton_{db} $\text{km}^2\text{year}^{-1}$, while for Norway, this value is only 5.2 ton_{db} $\text{km}^2\text{year}^{-1}$.

The emissions related to biomass transport per functional unit have been evaluated by multiplying the emissions related to the transport of 1 kg of dry-basis biomass to the feedstock demand to produce 1 MJ of SAF, specific for each route. As shown in the example below.

i.e. Austria (EtOH route) :

$$17.8 \frac{gCO_2}{kg_{db}} \cdot 0.1298 \frac{kg_{db}}{MJ_{SAF}} = 2.31 \frac{gCO_2}{MJ_{SAF}}$$

Figure 6.1: Country-based potential herbaceous crops production per square kilometer [51]
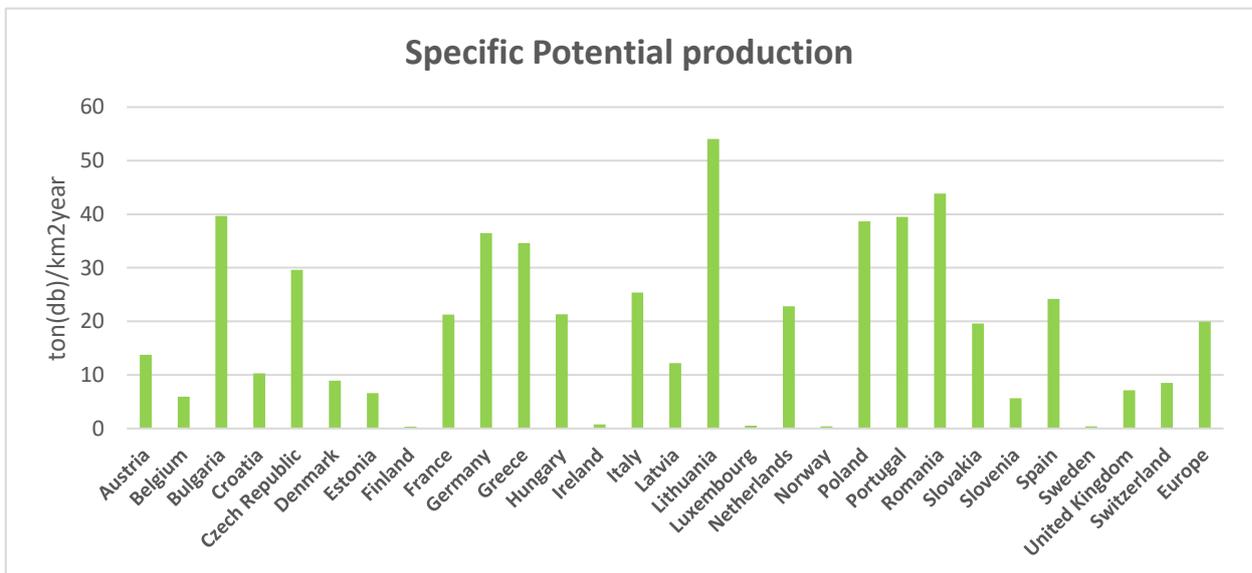
Figure 6.2: Country-based potential residues production per square kilometer [51]
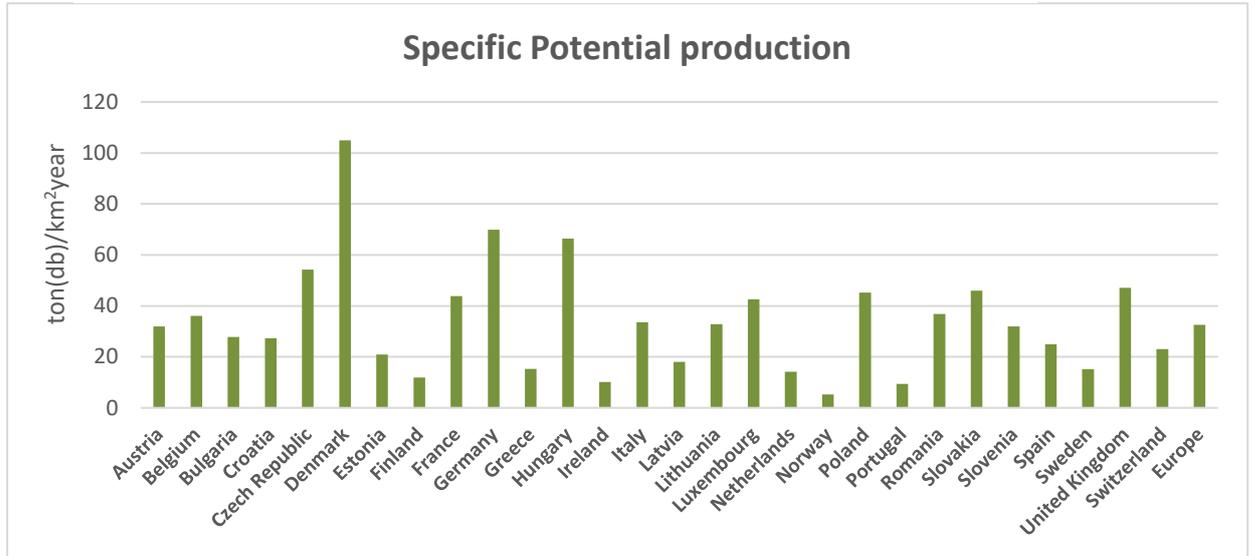
6.3 Electricity emission factor

As depicted in figure 6.3, the impact of 1 kWh of electricity in terms of emissions significantly varies depending on the public grid mix of the country. This value ranges from 19 gCO2eq/kWh in Norway to 976 gCO2eq/kWh in Poland, with a European average of 384 gCO2eq/kWh, based on data from ecoinvent [94]. Thus contributing to a large differentiation in the overall well-to-wings emissions among countries and routes.

The emissions related to electricity consumption per functional unit have been evaluated by multiplying the emissions related to the transport of 1 kWh of electricity to the electricity demand to produce 1 MJ of SAF, specific for each route. As shown in the example below.

i.e. Austria (EtOH route) : $\qquad 317 \frac{gCO_2}{kWh} \cdot 0.0213 \frac{kWh}{MJ_{SAF}} = 6.74 \frac{gCO_2}{MJ_{SAF}}$

Electricity emission factor
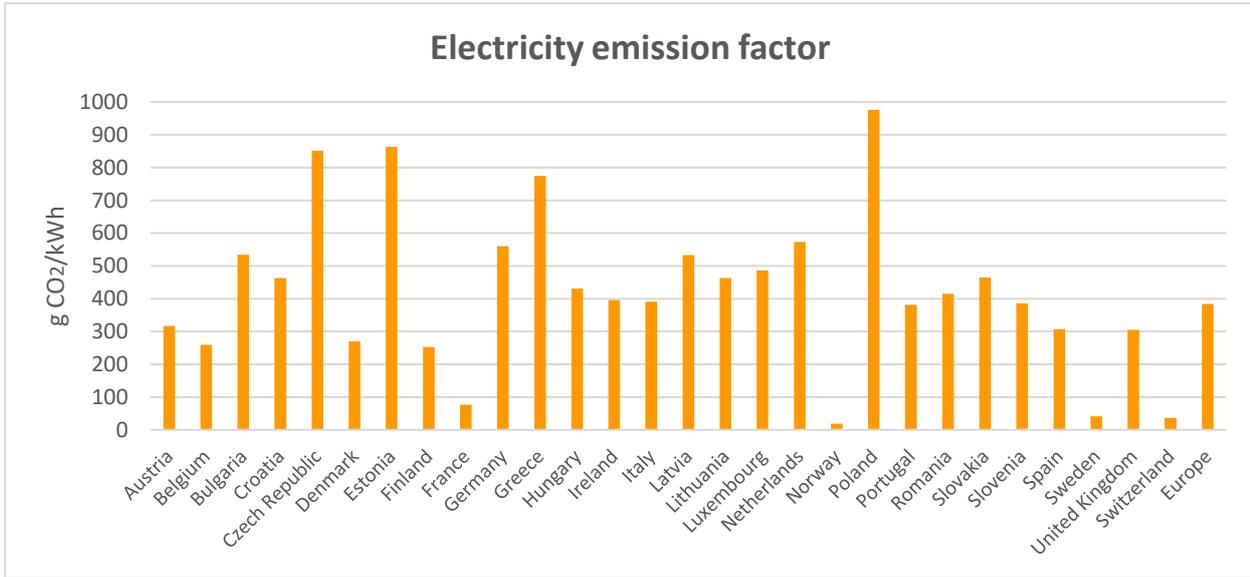
6.4 SAF transportation to airport

In order to discern the impact of transportation based on country-specific characteristics, such as size and aviation industry development, and in the absence of precise data, the specific airport distribution coefficient (α), was identified for each country. The coefficient is defined as the square root of the country's surface area, divided by the number of airports in that country and it provides a rough indication of the average distance between airports within a given country.

Subsequently, transport distances were categorized into three groups: 100 km if $0 \leq \alpha \leq 50$, 200 km if $50 < \alpha \leq 100$, and 300 km if $\alpha > 100$, aligning with the estimation obtained from literature [86]. Activity data for "market for transport, freight, lorry, unspecified", relative to Europe, was obtained from ecoinvent, providing the amount of CO_2 equivalent per ton-kilometer. The value correspond to 0.14871 $kgCO_2$ (ton km)$^{-1}$ thus, to assess the CO_2 equivalent per megajoule of SAF, relative to the transport distance from the biorefinery plant to the airport, the calculations were executed as follows:

- $1/LHV_{SAF} = 1/44 = 2.2727 \cdot 10^{-8} \, ton/MJ_{SAF}$: *mass of SAF per MJ, expressed in ton*
- $2.2727 \cdot 10^{-8} \cdot 0.14871 = 3.3798 \cdot 10^{-3} \, gCO_{2 \, eq}/km \cdot MJ_{SAF}$: *emissions per km·MJ, expressed in grams*

- $3{,}3798 \cdot 10^{-3} \cdot (100; 200; 300) = 0{,}3379\, CO_{2\,eq}/MJ_{SAF};\ 0{,}6759\, CO_{2\,eq}/MJ_{SAF};\ 1{,}014\, g\,CO_{2\,eq}/MJ_{SAF}$: *transportation emissions per MJ of SAF*

The obtained results fall within the order of magnitude of $1 g\,CO_2\ MJ_{SAF}^{-1}$, aligning with the amounts observed in comparable studies. As anticipated, its impact on the overall emissions across the entire Sustainable Aviation Fuel (SAF) supply chain is virtually negligible.

6.5 CORSIA supplementary scenario

To simulate this supplementary scenario, inventories for SAF though i-BuOH route were obtained from CORSIA Supporting Document [17] and are reported below. The simulation was performed in brightway 2 without excluding electricity input in order to assess only average results referred to Europe. The average emission factor concerning Europe was considered, taken from Ecoinvent 3.9, equal to 350 gCO_2 kWh^{-1}. The source for the MIT provided data is Staples et al. (2014) and the source for the JRC provided data is the E3 database (LudwigBolkow Systemtechnik GMBH, 2006). There are some differences in the results based on the MIT and JRC datasets. Feedstock transportation emissions from the JRC data (7.9 $gCO_2eq\ MJ_{SAF}^{-1}$) are higher than those from the MIT data (1.2 $gCO_2eq\ MJ_{SAF}^{-1}$), driven primarily by an assumption of greater transportation distances in the E3 database. In addition, differences in feedstock-to-fuel conversion are present, due to assumed net heat demand for fermentation of lignocellulosic feedstock to isobutanol (0.04 $MJ_{nat.gas}$ MJ_{SAF}^{-1} in MIT data versus 0.01 $MJ_{nat.gas}\ MJ_{SAF}^{-1}$ in JRC data), and the source and quantity of cellulase enzymes for bioconversion of lignocellulosic feedstock to isobutanol (0.85 $g_{cellulase}\ MJ_{SAF}^{-1}$ versus 1.62 $g_{cellulase}\ MJ_{SAF}^{-1}$). In the simulation conducted in this thesis only data from MIT were considered.

Figure 6.4: Lifecycle inventory for iso-butanol ATJ pathway [17]

Data provider			MIT	JRC
Corn stover collection and field treatment	Inputs	Diesel fuel [MJ/kgcorn stover]	0.30	0.17
		HDPE [g/kgcorn stover]	0.37	-
		Nitrogen [g/kgcorn stover]	8.77	9.61
		Phosphoric acid [g/kgcorn stover]	2.51	2.08
		Potassium Oxide [g/kgcorn stover]	15.04	15.77
Feedstock transportation	Inputs	Diesel fuel [MJ/kg corn stover]	0.11	7.5
Fermentation to iso-butanol	Inputs	Feedstock [kg/MJ$_{SAF}$]	0.15	0.16
		Natural gas for process heat [MJ/MJ$_{SAF}$]	0.03	0.01
		Cellulase [g/MJ$_{SAF}$]	1.4	0.84
		Yeast [g/MJ$_{SAF}$]	0.30	0
		Sulfuric acid [g/MJ$_{SAF}$]	4.1	3.69
		Ammonia [g/MJ$_{SAF}$]	2.7	2.23
		Sodium hydroxide [g/MJ$_{SAF}$]	-	4.06
		Calcium oxide [g/MJ$_{SAF}$]	-	1.64
		Corn steep liquor [g/MJ$_{SAF}$]	2.4	2.33
		Diammonium phosphate [g/MJ$_{SAF}$]	0.30	0.25
	Outputs	Co-produced electricity [kJ/MJ$_{SAF}$]	41.0	73.33
		iBuOH [g/MJ$_{SAF}$]	30.5	30.7
iBuOH upgrading to drop-in fuels	Inputs	iBuOH [g/MJ$_{SAF}$]	30.5	30.7
		Natural gas for process heat [MJ/MJ$_{SAF}$]	0.06	0.07
		Hydrogen [g/MJ$_{SAF}$]	0.19	0.2
	Outputs	Heavy oil [MJ/MJ$_{SAF}$]	0.03	-
		Naphtha [MJ/MJ$_{SAF}$]	-	0.22
		Diesel [MJ/MJ$_{SAF}$]	0.08	-
		Jet fuels [MJ/MJ$_{SAF}$]	1.0	1

Note: All corn stover is in units of dry biomass

The CORSIA modeling group thoroughly examined and compiled the life-cycle inventory for the Ethanol Alcohol-to-Jet (ATJ) process, sourcing information from various research papers and industry data, including Mei (2006), Braz et al. (2018), Crawford et al. (2016), Byogy, and LanzaTech. The focus of this section revolves around the fuel production pathway involving agricultural residues-derived ethanol, which undergoes conversion to drop-in fuel through dehydration, oligomerization, and hydrotreating. The system boundary encompasses feedstock collection, transportation to a drop-in fuel production facility, fermentation to ethanol, upgrading to a drop-in fuel slate, and the transportation and distribution of the finished jet fuel. Two ATJ conversion plant layouts, namely standalone and

integrated designs, are presented; however, this thesis exclusively refers to the standalone design.

Figure 6.5: Lifecycle inventory cellulosic ethanol ATJ pathway (agreed set of input between JRC and ANL) [17]

Ethanol production		Agricultural residues		Forest residues		Miscanthus		Switchgrass	
Inputs	Units	Standalone	Integrated	Standalone	Integrated	Standalone	Integrated	Standalone	Integrated
Biomass feedstock	dry kg	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
Natural gas	MJ	-	-	.042	.042	-	-	-	-
Diesel	MJ	0.0024	0.0024	.0044	.0044	0.0024	0.0024	0.0024	0.0024
Cellulase	g	1.33	1.33	1.33	1.33	1.33	1.33	1.33	1.33
Yeast	g	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
Sulfuric acid	g	4.30	4.30	4.30	4.30	4.30	4.30	4.30	4.30
Ammonia	g	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52
NaOH	g	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46
CaO	g	0.95	0.95	0.95	0.95	0.95	0.95	0.95	0.95
Corn steep liquor	g	1.63	1.63	1.63	1.63	1.63	1.63	1.63	1.63
DAP	g	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17
Urea	g	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26
Outputs									
Ethanol	MJ	1	1	1	1	1	1	1	1
Electricity before use for ATJ conversion	MJ	0.11	0.088	0.11	0.088	0.11	0.088	0.11	0.088

Ethanol-to-jet		Agricultural residues		Forest residues		Miscanthus		Switchgrass	
Inputs	Units	Standalone	Integrated	Standalone	Integrated	Standalone	Integrated	Standalone	Integrated
Ethanol	MJ	1.06	1.06	1.06	1.06	1.06	1.06	1.06	1.06
Hydrogen	MJ	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06
Natural gas	MJ	0.18	0	0.18	0	0.18	0	0.18	0
Electricity	MJ	0.02	0	0.02	0	0.02	0	0.02	0
Total Energy Input	**MJ**	**1.32**	**1.12**	**1.32**	**1.12**	**1.32**	**1.12**	**1.32**	**1.12**
Outputs									
Jet fuel and other energy products	MJ	1	1	1	1	1	1	1	1

6.8 Well-to-wings country-based emissions per each scenarios

Table 6.1: Well-to-wings emissions - Herbaceous energy crops, EtOH route

Country	Ethanol to jet							
	Feedstock demand	Biomass production	Biomass transport	Electricity from the grid		Industrial convertion - without elect.	Jet fuel transport	Feed to jet
	kg db / MJ SAF	gCO₂eq/MJ SAF	gCO₂eq/MJ SAF	kWh/MJ SAF	g CO2/MJ SAF	g CO2/MJ SAF	gCO₂eq/MJ SAF	gCO₂eq/MJ SAF
Austria	0.130	21.15	2.31	0.021	6.74	18.14	1.35	49.70
Belgium	0.130	21.15	3.51	0.021	5.51	18.14	1.35	49.66
Bulgaria	0.130	21.15	1.36	0.021	11.36	18.14	1.01	53.03
Croatia	0.130	21.15	2.66	0.021	9.85	18.14	1.35	53.15
Czechia	0.130	21.15	1.57	0.021	18.12	18.14	1.01	60.00
Denmark	0.130	21.15	2.86	0.021	5.74	18.14	1.01	48.91
Estonia	0.130	21.15	3.32	0.021	18.36	18.14	1.35	62.32
Finland	0.130	24.36	14.75	0.021	5.38	18.14	1.35	63.98
France	0.130	21.15	1.67	0.021	1.62	18.14	1.01	43.60
Germany	0.130	21.15	1.42	0.021	11.91	18.14	1.01	53.63
Greece	0.130	21.15	1.45	0.021	16.48	18.14	1.35	58.58
Hungary	0.130	21.15	1.86	0.021	9.17	18.14	1.35	51.67
Ireland	0.130	21.15	9.70	0.021	8.42	18.14	1.35	58.77
Italy	0.130	21.15	1.70	0.021	8.32	18.14	1.35	50.66
Latvia	0.130	21.15	2.44	0.021	11.34	18.14	1.35	54.42
Lithuania	0.130	21.15	1.17	0.021	9.85	18.14	1.01	51.32
Luxembourg	0.130	21.15	11.74	0.021	10.34	18.14	1.01	62.38
Netherlands	0.130	21.15	1.70	0.021	12.19	18.14	1.01	54.20
Norway	0.130	24.36	12.92	0.021	0.40	18.14	1.35	57.17
Poland	0.130	21.15	1.38	0.021	20.76	18.14	1.35	62.78
Portugal	0.130	17.35	1.34	0.021	8.10	18.14	1.69	46.62
Romania	0.130	21.15	1.29	0.021	8.83	18.14	1.69	51.09
Slovakia	0.130	21.15	1.93	0.021	9.89	18.14	1.35	52.47
Slovenia	0.130	21.15	3.60	0.021	8.21	18.14	1.35	52.45
Spain	0.130	21.15	1.73	0.021	6.53	18.14	1.35	48.90
Sweden	0.130	24.36	13.31	0.021	0.87	18.14	1.35	58.03
U.K.	0.130	21.15	3.22	0.021	6.49	18.14	1.01	50.01
Switzerland	0.130	21.15	2.87	0.021	0.77	18.14	1.01	43.94
Europe	0.130	21.36	3.96	0.021	8.17	18.14	1.35	52.98

Table 6.2: Well-to-wings emissions - Herbaceous energy crops. i-BuOH route

Country	Isobutanol to jet							
	Feedstock demand	Biomass production	Biomass transport	Electricity from the grid		Industrial convertion - without elect.	Jet fuel transport	Feed to jet
	kg db / MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF	kWh/MJ SAF	g CO2/MJ SAF	g CO2/MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF
Austria	0.132	21.49	2.35	0.005	1.67	19.84	0.34	45.70
Belgium	0.132	21.49	3.56	0.005	1.37	19.84	0.68	46.94
Bulgaria	0.132	21.49	1.39	0.005	2.82	19.84	1.01	46.56
Croatia	0.132	21.49	2.70	0.005	2.44	19.84	0.68	47.16
Czechia	0.132	21.49	1.60	0.005	4.50	19.84	0.34	47.77
Denmark	0.132	21.49	2.90	0.005	1.43	19.84	0.34	46.01
Estonia	0.132	21.49	3.38	0.005	4.55	19.84	0.68	49.95
Finland	0.132	24.75	14.99	0.005	1.34	19.84	0.68	61.60
France	0.132	21.49	1.70	0.005	0.40	19.84	0.34	43.78
Germany	0.132	21.49	1.44	0.005	2.96	19.84	0.34	46.07
Greece	0.132	21.49	1.48	0.005	4.09	19.84	0.68	47.58
Hungary	0.132	21.49	1.89	0.005	2.27	19.84	0.68	46.18
Ireland	0.132	21.49	9.86	0.005	2.09	19.84	0.68	53.96
Italy	0.132	21.49	1.73	0.005	2.06	19.84	0.68	45.81
Latvia	0.132	21.49	2.48	0.005	2.81	19.84	0.68	47.31
Lithuania	0.132	21.49	1.19	0.005	2.44	19.84	0.34	45.31
Luxembourg	0.132	21.49	11.93	0.005	2.57	19.84	1.01	56.85
Netherlands	0.132	21.49	1.73	0.005	3.02	19.84	0.34	46.43
Norway	0.132	24.75	13.13	0.005	0.10	19.84	0.68	58.50
Poland	0.132	21.49	1.40	0.005	5.15	19.84	0.68	48.57
Portugal	0.132	17.63	1.36	0.005	2.01	19.84	1.01	41.86
Romania	0.132	21.49	1.31	0.005	2.19	19.84	1.01	45.85
Slovakia	0.132	21.49	1.97	0.005	2.45	19.84	0.68	46.44
Slovenia	0.132	21.49	3.66	0.005	2.04	19.84	0.68	47.71
Spain	0.132	21.49	1.75	0.005	1.62	19.84	0.68	45.39
Sweden	0.132	24.75	13.52	0.005	0.22	19.84	0.68	59.02
U.K.	0.132	21.49	3.27	0.005	1.61	19.84	0.34	46.56
Switzerland	0.132	21.49	2.92	0.005	0.19	19.84	0.34	44.78
Europe	0.132	21.71	4.02	0.005	2.03	19.84	0.68	48.27

Table 6.3: Well-to-wings emissions - Herbaceous energy crops. IBN route

Country	Isobutane to jet							
	Feedstock demand	Biomass production	Biomass transport	Electricity from the grid		Industrial convertion - without elect.	Jet fuel transport	Feed to jet
	kg db / MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF	kWh/MJ SAF	g CO2/MJ SAF	g CO2/MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF
Austria	0.117	19.12	2.09	0.077	24.47	12.48	0.34	58.49
Belgium	0.117	19.12	3.17	0.077	19.99	12.48	0.68	55.44
Bulgaria	0.117	19.12	1.23	0.077	41.22	12.48	1.01	75.06
Croatia	0.117	19.12	2.41	0.077	35.74	12.48	0.68	70.42
Czechia	0.117	19.12	1.42	0.077	65.77	12.48	0.34	99.12
Denmark	0.117	19.12	2.58	0.077	20.84	12.48	0.34	55.36
Estonia	0.117	19.12	3.00	0.077	66.61	12.48	0.68	101.89
Finland	0.117	22.02	13.33	0.077	19.53	12.48	0.68	68.04
France	0.117	19.12	1.51	0.077	5.87	12.48	0.34	39.32
Germany	0.117	19.12	1.28	0.077	43.23	12.48	0.34	76.44
Greece	0.117	19.12	1.31	0.077	59.82	12.48	0.68	93.41
Hungary	0.117	19.12	1.68	0.077	33.27	12.48	0.68	67.22
Ireland	0.117	19.12	8.77	0.077	30.57	12.48	0.68	71.61
Italy	0.117	19.12	1.54	0.077	30.18	12.48	0.68	63.99
Latvia	0.117	19.12	2.21	0.077	41.14	12.48	0.68	75.62
Lithuania	0.117	19.12	1.06	0.077	35.74	12.48	0.34	68.73
Luxembourg	0,117	19,12	10,61	0,077	37,51	12.48	1.01	80,74
Netherlands	0,117	19,12	1.54	0,077	44,23	12.48	0.34	77,70
Norway	0,117	22.02	11.68	0,077	1.47	12.48	0,68	48,32
Poland	0,117	19,12	1.24	0,077	75,34	12.48	0.68	108,86
Portugal	0,117	15,68	1.21	0,077	29,41	12.48	1.01	59,79
Romania	0,117	19,12	1.16	0,077	32.03	12.48	1.01	65,81
Slovakia	0,117	19,12	1.75	0,077	35,89	12.48	0.68	69,92
Slovenia	0,117	19,12	3,25	0,077	29,80	12.48	0.68	65,32
Spain	0.117	19.12	1.56	0.077	23.70	12.48	0.68	57.53
Sweden	0.117	22.02	12.03	0.077	3.16	12.48	0.68	50.37
U.K.	0.117	19.12	2.91	0.077	23.54	12.48	0.34	58.39
Switzerland	0.117	19.12	2.59	0.077	2.78	12.48	0.34	37.31
Europe	0.117	19.31	3.58	0.077	29.64	12.48	0.68	65.68

Table 6.4: Well-to-wings emissions - residues. EtOH route

Country	Ethanol to jet						
	Feedstock demand	Biomass transport	Electricity from the grid		Industrial convertion without elect.	Jet fuel transport	Feed to jet
	kg db / MJ SAF	g CO2/MJ SAF	kWh/MJ SAF	g CO2/MJ SAF	g CO2/MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF
Austria	0.130	1.27	0.021	6.74	18.14	0.34	26.50
Belgium	0.130	1.20	0.021	5.51	18.14	0.68	25.53
Bulgaria	0.130	1.35	0.021	11.36	18.14	1.01	31.87
Croatia	0.130	1.39	0.021	9.85	18.14	0.68	30.06
Czechia	0.130	0.97	0.021	18.12	18.14	0.34	37.57
Denmark	0.130	0.68	0.021	5.74	18.14	0.34	24.90
Estonia	0.130	1.54	0.021	18.36	18.14	0.68	38.72
Finland	0.130	1.99	0.021	5.38	18.14	0.68	26.19
France	0.130	0.98	0.021	1.62	18.14	0.34	21.08
Germany	0.130	0.85	0.021	11.91	18.14	0.34	31.24
Greece	0.130	1.83	0.021	16.48	18.14	0.68	37.14
Hungary	0.130	0.89	0.021	9.17	18.14	0.68	28.88
Ireland	0.130	2.26	0.021	8.42	18.14	0.68	29.50
Italy	0.130	1.24	0.021	8.32	18.14	0.68	28.37
Latvia	0.130	1.66	0.021	11.34	18.14	0.68	31.82
Lithuania	0.130	1.24	0.021	9.85	18.14	0.34	29.57
Luxembourg	0.130	1.08	0.021	10.34	18.14	1.01	30.58
Netherlands	0.130	1.74	0.021	12.19	18.14	0.34	32.41
Norway	0.130	3.09	0.021	0.40	18.14	0.68	22.31
Poland	0.130	1.06	0.021	20.76	18.14	0.68	40.64
Portugal	0.130	2.36	0.021	8.10	18.14	1.01	29.62
Romania	0.130	1.18	0.021	8.83	18.14	1.01	29.16
Slovakia	0.130	1.06	0.021	9.89	18.14	0.68	29.77
Slovenia	0.130	1.27	0.021	8.21	18.14	0.68	28.30
Spain	0.130	1.45	0.021	6.53	18.14	0.68	26.80
Sweden	0.130	1.78	0.021	0.87	18.14	0.68	21.47
U.K.	0.130	1.06	0.021	6.49	18.14	0.34	26.03
Switzerland	0.130	1.47	0.021	0.77	18.14	0.34	20.71
Europe	0.130	1.24	0.021	8.17	18.14	0.68	28.22

Table 6.5: Well-to-wings emissions - residues. i-BuOH route

Country	Isobutanol to jet						
	Feedstock demand	Biomass transport	Electricity from the grid		Industrial convertion without elect.	Jet fuel transport	Feed to jet
	kg db / MJ SAF	g CO2/MJ SAF	kWh/MJ SAF	g CO2/MJ SAF	g CO2/MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF
Austria	0.132	1.30	0.005	1.67	19.84	0.34	23.15
Belgium	0.132	1.22	0.005	1.37	19.84	0.68	23.10
Bulgaria	0.132	1.37	0.005	2.82	19.84	1.01	25.05
Croatia	0.132	1.41	0.005	2.44	19.84	0.68	24.38
Czechia	0.132	0.98	0.005	4.50	19.84	0.34	25.66
Denmark	0.132	0.69	0.005	1.43	19.84	0.34	22.29
Estonia	0.132	1.57	0.005	4.55	19.84	0.68	26.65
Finland	0.132	2.02	0.005	1.34	19.84	0.68	23.88
France	0.132	1.00	0.005	0.40	19.84	0.34	21.58
Germany	0.132	0.86	0.005	2.96	19.84	0.34	24.00
Greece	0.132	1.86	0.005	4.09	19.84	0.68	26.48
Hungary	0.132	0.90	0.005	2.27	19.84	0.68	23.70
Ireland	0.132	2.30	0.005	2.09	19.84	0.68	24.91
Italy	0.132	1.26	0.005	2.06	19.84	0.68	23.84
Latvia	0.132	1.69	0.005	2.81	19.84	0.68	25.02
Lithuania	0.132	1.26	0.005	2.44	19.84	0.34	23.88
Luxembourg	0.132	1.10	0.005	2.57	19.84	1.01	24.52
Netherlands	0.132	1.77	0.005	3.02	19.84	0.34	24.97
Norway	0.132	3.14	0.005	0.10	19.84	0.68	23.76
Poland	0.132	1.08	0.005	5.15	19.84	0.68	26.75
Portugal	0.132	2.39	0.005	2.01	19.84	1.01	25.26
Romania	0.132	1.20	0.005	2.19	19.84	1.01	24.25
Slovakia	0.132	1.08	0.005	2.45	19.84	0.68	24.05
Slovenia	0.132	1.30	0.005	2.04	19.84	0.68	23.85
Spain	0.132	1.47	0.005	1.62	19.84	0.68	23.61
Sweden	0.132	1.81	0.005	0.22	19.84	0.68	22.54
U.K.	0.132	1.08	0.005	1.61	19.84	0.34	22.87
Switzerland	0.132	1.49	0.005	0.19	19.84	0.34	21.86
Europe	0.132	1.26	0.005	2.03	19.84	0.68	23.80

Table 6.6: Well-to-wings emissions - residues. IBN route

Country	Isobutene to jet						
	Feedstock demand	Biomass transport	Electricity from the grid		Industrial convertion without elect.	Jet fuel transport	Feed to jet
	kg db / MJ SAF	gCO2eq/MJ SAF	kWh/MJ SAF	g CO2/MJ SAF	g CO2/MJ SAF	gCO2eq/MJ SAF	gCO2eq/MJ SAF
Austria	0.117	1.15	0.077	24.47	12.48	0.34	38.44
Belgium	0.117	1.08	0.077	19.99	12.48	0.68	34.23
Bulgaria	0.117	1.22	0.077	41.22	12.48	1.01	55.93
Croatia	0.117	1.26	0.077	35.74	12.48	0.68	50.15
Czechia	0.117	0.87	0.077	65.77	12.48	0.34	79.46
Denmark	0.117	0.61	0.077	20.84	12.48	0.34	34.27
Estonia	0.117	1.40	0.077	66.61	12.48	0.68	81.17
Finland	0.117	1.80	0.077	19.53	12.48	0.68	34.48
France	0.117	0.89	0.077	5.87	12.48	0.34	19.57
Germany	0.117	0.77	0.077	43.23	12.48	0.34	56.81
Greece	0.117	1.66	0.077	59.82	12.48	0.68	74.64
Hungary	0.117	0.80	0.077	33.27	12.48	0.68	47.23
Ireland	0.117	2.04	0.077	30.57	12.48	0.68	45.76
Italy	0.117	1.12	0.077	30.18	12.48	0.68	44.45
Latvia	0.117	1.50	0.077	41.14	12.48	0.68	55.80
Lithuania	0.117	1.12	0.077	35.74	12.48	0.34	49.67
Luxembourg	0.117	0.98	0.077	37.51	12.48	1.01	51.98
Netherlands	0.117	1.57	0.077	44.23	12.48	0.34	58.62
Norway	0.117	2.79	0.077	1.47	12.48	0.68	17.41
Poland	0.117	0.96	0.077	75.34	12.48	0.68	89.45
Portugal	0.117	2.13	0.077	29.41	12.48	1.01	45.03
Romania	0.117	1.06	0.077	32.03	12.48	1.01	46.59
Slovakia	0.117	0.96	0.077	35.89	12.48	0.68	50.01
Slovenia	0.117	1.15	0.077	29.80	12.48	0.68	44.10
Spain	0.117	1.31	0.077	23.70	12.48	0.68	38.16
Sweden	0.117	1.61	0.077	3.16	12.48	0.68	17.93
U.K.	0.117	0.96	0.077	23.54	12.48	0.34	37.32
Switzerland	0.117	1.33	0.077	2.78	12.48	0.34	16.92
Europe	0.117	1.12	0.077	29.64	12.48	0.68	43.91

6.8 Scale-up potential to meet the forecasted aviation fuel demand

To evaluate the anticipated jet fuel demand in 2025, the International Energy Agency (IEA) estimated it to be equivalent to the pre-pandemic level [4]. Consequently, data for the year 2019 was considered as a basis for this estimation evaluated in Millions of barrels per year (Mbpy). Taking into consideration the overall availability of residues from N. Scarlat et al. [20] and the cultivation of herbaceous crops in marginal lands, as provided by Watanabe [51] and outlined in the subsequent table, the annual potential production of ATJ-based SAF was evaluated. This involved dividing the yearly biomass availabilities by the feedstock demand of the selected ATJ pathway. The results were then converted into millions of barrels (Mb) with the conversion factor 1 barrel = 158.987 liter.

i.e. Austria (H.C.): $1152.6 \frac{kton_{db}}{year} \cdot \frac{1}{0.157} \frac{MJ_{SAF}}{kg_{db}} \cdot \frac{1}{44} \frac{kg_{SAF}}{MJ_{SAF}} \cdot \frac{1}{0.821} \frac{l_{SAF}}{kg_{SAF}} \cdot \frac{1}{158.9} \frac{Mb}{l_{SAF}} =$ $1.28 \; Mbpy$

The i-BuOH pathway emerged as the preferred choice for all countries due to its highest evaluated yield per 100 kg of biomass (2.8 kg, compared to 2.13 kg and 1.41 kg for ethanol and isobutene, respectively). The corresponding feedstock demand was estimated at $0.157 \; kg_{db} \; MJ_{SAF}^{-1}$. The percentage of SAF supply to meet the fossil jet fuel demand was computed by dividing the annual potential ATJ-based SAF production (from Residues + Herbaceous crops) by the current jet fuel demand.

i.e. Austria: $(1.28 \; Mbpy + 2.97 \; Mbpy)/7.7 \; Mbpy$

With reference on the trade-scenario additional kerosene to cover the SAF shortage was evaluated for each country by subtracting the current jet fuel demand per the potential SAF production with full exploitation of country feedstock.

i.e. Austria: $7.7 \; Mbpy - (1.28 \; Mbpy + 2.97 \; Mbpy) = 3.4 Mbpy$

i.e. Romania: $1.5 \; Mbpy - (11.6 \; Mbpy + 9.7 \; Mbpy) = -19.9 Mbpy$

The estimated emissions concerning SAF production plus the additional kerosene demand (which in some cases is negative due to biomass over availability) were

computed by using the emission factor per functional unit specific for each scenario, such as residues, herbaceous crops, and kerosene.

i.e. Austria: $17.1 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 23.2 \frac{g_{CO2eq}}{MJ_{SAF}} + 7.4 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 45.7 \frac{g_{CO2eq}}{MJ_{SAF}} +$

$$19.7 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 94 \frac{g_{CO2eq}}{MJ_{SAF}} = 2573.9 kton_{CO2eq}$$

i.e. Romania: $55.9 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 24.2 \frac{g_{CO2eq}}{MJ_{SAF}} + 66.7 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot$

$$46.3 \frac{g_{CO2eq}}{MJ_{SAF}} - 114.2 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 94 \frac{g_{CO2eq}}{MJ_{SAF}} = -6322.3 kton_{CO2eq}$$

<u>Emission share respect to the baseline</u>

i.e. Austria: $\frac{2573.9 kton_{CO2eq}}{4138.1 kton_{CO2eq}} = 62.2\%$

i.e. Romania: $\frac{-6322.3 kton_{CO2eq}}{788.2 kton_{CO2eq}} = -802.1\%$

Climate change mitigation potential share was defined as the reduction in emissions resulting from the utilization of SAF, compared to the baseline scenario, assessed by multiplying the projected jet fuel demand values by the baseline of 94 gCO$_2$eq MJ^{-1}.

i.e. Austria: $\left(1 - \frac{2573.9 kton_{CO2eq}}{4138.1 kton_{CO2eq}} \right) \cdot 100 = 38.8\%$

i.e. Romania: $\left(1 - \frac{2573.9 kton_{CO2eq}}{4138.1 kton_{CO2eq}} \right) \cdot 100 = 902.2\%$

To estimate SAF production for each country to fulfill fuel demand in non-trading scenario, residues were prioritized. If their contribution proved insufficient, herbaceous crops were considered. If SAF production still fell short of covering the jet fuel demand, the gap was filled with kerosene fuel. The estimated emissions were then computed based on the respective emission factors for each scenario.

Estimated emissions with ATJ SAF introduction

i.e. Austria: $17.1 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 23.2 \frac{g_{CO2eq}}{MJ_{SAF}} + 7.4 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 45.7 \frac{g_{CO2eq}}{MJ_{SAF}} +$

$19.7 \frac{MJ_{SAF} \cdot kton_{CO2eq}}{g_{CO2eq}} \cdot 94 \frac{g_{CO2eq}}{MJ_{SAF}} = 2573.9 kton_{CO2eq}$

Emission share respect to the baseline

i.e. Austria: $\frac{2573.9 kton_{CO2eq}}{4138.1 kton_{CO2eq}} = 62.2\%$

Climate change mitigation potential share was defined as the reduction in emissions resulting from the utilization of SAF, compared to the baseline scenario, assessed by multiplying the projected jet fuel demand values by the baseline of 94 gCO$_2$eq MJ^{-1}.

i.e. Austria: $1 - \frac{2573.9 kton_{CO2eq}}{4138.1 kton_{CO2eq}} = 38.8\%$

Table 6.7: Country-based potential residues and energy crops availability [20] [51]

Country	Herbaceous crops cultivated in marginal lands		Agricultural residues	Forest residues	Total residues
	kton(db)/year		kton(db)/year	kton(db)/year	kton(db)/year
Austria	Switchgrass	1152.6	1026	1650	2676
Belgium	Switchgrass	182.3	884	217	1101
Bulgaria	Switchgrass	4406.4	2643	448	3091
Croatia	Switchgrass	581.9	1160	384	1544
Czechia	Switchgrass	2337.5	3004	1271	4275
Denmark	Switchgrass	384.5	4340	186	4526
Estonia	Switchgrass	299.9	311	635	946
Finland	Reed canary	113.8	1348	2680	4028
France	Switchgrass	14380.2	24684	4905	29589
Germany	Switchgrass	13040.5	20682	4312	24994
Greece	Switchgrass	4569.2	1751	273	2024
Hungary	Switchgrass	1982.8	5548	627	6175
Ireland	Switchgrass	54.4	518	192	710
Italy	Switchgrass	7660.2	8772	1379	10151
Latvia	Switchgrass	789	189	979	1168
Lithuania	Switchgrass	3524.3	1636	507	2143
Luxembourg	Switchgrass	1.4	51	59	110
Netherlands	Switchgrass	946.6	510	80	590
Norway	Reed canary	160	528	1478	2006
Poland	Switchgrass	12094.4	11743	2392	14135
Portugal	Miscanthus	3651.7	401	466	867
Romania	Switchgrass	10454.7	7009	1758	8767
Slovakia	Switchgrass	961.6	1695	557	2252
Slovenia	Switchgrass	114.8	162	486	648
Spain	Switchgrass	12215.2	11239	1324	12563
Sweden	Reed canary	184.9	2115	4713	6828
U.K.	Switchgrass	1730.2	10106	1314	11420
Switzerland	Switchgrass	350.6	312	640	952
Europe	/	3511.6	124367	35912	160279