



Aviation fuel production pathways from lignocellulosic biomass via alcohol intermediates – A technical analysis

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ABSTRACT

In order to achieve the goal of limiting global warming to 1.5 °C, also the growing aviation industry needs to take measures to reduce their greenhouse gas emissions. Various renewably sourced aviation fuels can significantly reduce greenhouse gas emissions and most of them, except for example liquid hydrogen or LNG, can be used in the existing infrastructure without airport or aircraft modifications. As most of these renewably sourced fuel types are not (yet) produced at commercial scale, many technological assessment parameter (e.g. carbon or energy efficiency) are uncertain. Thus, the goal of this study is to compare two different process routes, both being based on biochemical and thermochemical conversion steps. The processes evaluated against conversion efficiency of the available raw feedstock and process energy requirements. The evaluation uses theoretical and biochemical carbon efficiency as well as energy efficiency as indicators. A steady-state flowsheet simulation for two biogenic process paths via biogas and bioethanol as intermediate products is carried out on the basis of literature data. In addition, the optional use of solid residue from the biotechnological process step by combustion for direct heat supply cases are studied. In the ethanol-based route, about 23% of the carbon in the feed can be recovered as kerosene, whereas this is only about 19% in the biogas route. Simultaneously, the ethanol-based route without the combustion of the residue has an energy efficiency of 28%, while the biogas route has an efficiency of 24%.

1. Introduction

In order to limit global warming to a global average temperature increase well below 2 °C and take action to limit it to 1.5 °C (i.e., to comply with the Paris Agreement [1]), all sectors must substantially contribute to reduce the greenhouse gas (GHG) emissions. Both, the International Air Transport Association (IATA) and the International Civil Aviation Organisation (ICAO), have announced a reduction target for GHG emissions from commercial aviation to net zero by 2050 [2]. With an average long-term air traffic growth rate of around 4% a⁻¹ and a simultaneous reduction in passenger-specific fuel consumption of 1.3% a⁻¹, effective measures exceeding clearly the already implemented actions must be taken to fulfil these demanding reduction goals [3,4]. Furthermore, there is an increasing relevance and also strong need to consider and reduce non-CO₂ climate relevant effects in addition to the GHG emissions of aviation in order to achieve a climate neutral civil aviation in the years to come [5–9].

Various technical, operational and infrastructural possibilities are given to reduce the GHG emissions in air traffic. One option is to replace

the currently used fossil-based aviation fuel with a renewable sourced energy carrier [10]. This could, for instance, involve the use of a liquid energy carrier with substantial different chemical properties compared to fossil fuel-based aviation fuels (“non-drop in fuels”) or even electrically powered aircrafts. Such options are characterized by a high potential not only for reducing CO₂ resp. GHG-related effects, but also for lowering non-CO₂ effects [11–13]. In turn, for their implementation within the civil aviation sector the development and construction of completely new aircraft, fuel / energy supply infrastructure would be necessary and, under the current state of research, would also be linked to a limitation of the payload or range [14,15].

In contrast, there is the possibility of replacing the currently used fossil fuel-based kerosene with fuels which show almost identical chemical properties (“drop-in fuels”). Such a “green” kerosene fuel, usually referred to as Sustainable Aviation Fuel (SAF), is chemically widely similar to the fossil fuel-based comparative and thus offers the possibility of refuelling the aircraft fleet with an almost CO₂-neutral aviation fuel. In theory, such a strategy can be realized on relatively short notice by using basically the same fuel supply infrastructure as

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well as the same aeroplane fleet.

At present, seven different production processes are approved by ASTM being the responsible fuel standardisation body and can therefore be used to provide SAF. These alternative fuel components / the respective SAF must then be blended with at least 50% fossil fuel-based kerosene to meet the requirements of the currently valid ASTM D7566 and the D1655 [16,17]. In doing so, such SAF-blended fuels can halve the CO₂ emissions from air traffic; additionally, they can also contribute to reduce non-CO₂ effects on climate by adjusting the fuel composition within the limits defined by the standards mentioned above [18–20]. If the currently valid standards are adjusted in the years to come to allow also a 100% usage of SAF (being necessary anyway to fulfil the legal GHG reduction goals) the GHG emissions from civil aviation can be reduced to net zero in theory.

Today, SAF can be produced from various biogenic and non-biogenic sources via biochemical or thermochemical processes or a combination of these. The common goal of these partly very different processes is to produce a SAF directly usable with the current fossil fuel-based kerosene infrastructure (i.e., drop-in fuel). A distinction can be made between production processes which do not use biomass-based feedstock (except biogenic CO₂) commonly referred to as renewable fuels of non-biological origin (RFNBO or also known as e-fuels) and those utilizing exclusively biological feedstock (i.e., biomass). Subsequently, RFNBOs are primarily based on the use of electricity from renewable sources of energy and bind this energy resource materially with the help of CO₂ and H₂O [21]. Production volumes of RFNBO are thus constrained by the available generation capacities of renewably sourced electricity and the large-scale infrastructure for material inputs like hydrogen from water electrolysis and CO from CO₂ reduction [22,23].

In contrast to RFNBOs, fuels and energy carriers from biogenic sources are already produced in large quantities today on a global scale. In addition to vegetable oils from various sources (also: used cooking oil (UCO)), biogas and bioethanol are also available as “green” molecules used today in particular for heat and/or electricity generation as well as for road transport. Biogas and bioethanol, however, cannot be fuelled as a direct drop-in capable fuel into an commercial aircraft, and also show disadvantageous fuel properties compared to drop-in capable aviation fuels [14,24].

Today’s global bioethanol production is around 100 Mt a⁻¹ (2670 PJ), for which an extensive infrastructure already exists. Currently, a large part of the world-wide ethanol production is used as a biogenic fuel component to be added into fossil-fuel based gasoline used in road transport. In parallel, further processing of these “green” ethanol molecules into various other fuel products is being discussed; in this context, the conversion into SAF is also being considered [25]. Starting from such a bio-based alcohol, with so called Alcohol-to-Jet (AtJ) processes a conversion into a SAF is possible. This process route, based on ethanol or on isobutanol, is one of the seven process routes already approved by ASTM (ASTM D7566) [17]. Additionally, first demonstration plants are being built with a production volume of around 30 kt a⁻¹ [26].

Biogas is produced globally from agricultural biomass as well as organic residue and waste streams in large volumes equivalent to 1100 PJ in 2020 [27]. This biogas is either used directly or separated from CO₂ and used as biomethane e.g., within road traffic applications. For its potential use as a kerosene-like SAF, biogas must first be converted via an intermediate step to a synthesis gas to be further processed either to methanol and the further via the Methanol-to-Jet (MtJ) route or via the Fischer Tropsch (FT) route to a kerosene-like SAF. In contrast to the MtJ route, the FT route is already approved within the ASTM D7566 [17]. In turn, the advantage of the MtJ route is that methanol is already – in contrast to FT crude – a globally traded commodity, even if production today mainly relies on fossil resources [28,29].

Process routes based on biogas and bioethanol require biotechnologically produced intermediate products based on biomass as a feedstock. If the biomass feedstock needed for the provision of these intermediates competes with the food and fodder market, within the

global population an increasing concern is emerging about possibly rising food prices due to a globally increasing food demand of a growing population and decreasing fertile land due to climate change and a strong expansion of urban areas. Additionally, environmental concerns were raised about the increasing cultivation of biomass [30,31]. Using organic waste streams / biomass residues / agricultural by-products (e.g., straw) or lignocellulosic biomass can alleviate the impact on these parameters [32]. Nevertheless, fertile land is limited and thus a compromise needs to be found between the use of this land for food provision, for the production of biogenic raw materials for industry and commerce, the provision of energy and/or landscape preservation and biodiversity conservation. The use of biomass additionally also has a direct climate impact, such as the clearing of rainforests.

Against this background, the overarching aim of the paper is to technically compare two kerosene production processes which both utilize lignocellulosic biomass and biotechnologically produced intermediate products. As a possible widely available agricultural by-product, corn stover is assumed as the used feedstock, as it could be made available in potentially substantial quantities. The production processes are selected in a way that their intermediates are already available on the world markets in order to lower dependency on the development of individual process steps in the respective process chain. This is the case for both ethanol and biogas or methanol intermediate, which is why the process development is based on these intermediate products. Each process is additionally designed to achieve the highest possible carbon use efficiency, while abstaining from using large-scale electrolysis for further carbon reduction. Hence, the focus remains on primarily biogenic fuels.

To achieve this overarching goal this paper is structured as follows. First, the foundation is laid by a characterization of the feedstock used and the possible conversion processes. Next, the methods used to design the specific processes and to analyse them are described. Following this approach, the processes are described and subsequently evaluated. Finally, the results are summarized and an outlook is provided.

2. Fundamentals

In the following, the basics of providing SAF from biogenic sources are outlined. The feedstock is described in detail before the biochemical and thermochemical processes for conversion are presented separately.

2.1. Feedstock

Feedstock containing high concentrations of lignocellulose are of particular interest, as they can serve as a source of carbon and energy and being widely available (e.g., straw) in various parts of our world [33]. Additionally, lignocellulosic biomass is selected here in such a way, that it allows to produce an advanced biofuel in accordance with the valid European directives [21]. Such lignocellulosic biomass mainly contains 12 to 25 wt% lignin, 30 to 50 wt% cellulose and 20 to 35 wt% hemicellulose. In addition, various other components (e.g., inorganic biomass components, proteins, soil particles) might be present in smaller proportions [34].

Table 1 shows exemplarily the composition of the feedstock corn stover assumed here. Extractives include various components that are soluble in either water or ethanol. Thus, corn stover vary widely in composition and moisture content. The latter depends on several external factors such as weather, soil quality, harvesting, and storage. In addition to the main atomic components carbon, hydrogen and oxygen, such biomass contains also sulphur and nitrogen [35].

When using lignocellulosic feedstock as a by-product from agricultural production, typically only a part of this biomass (e.g., straw) can be used in a sustainable way. Typically, a certain share of this biomass must remain on the field to reintroduce nutrients and to maintain the humus content of the soil. As a rule of thumb, typically roughly 50% of the biomass can be removed from the agricultural production system in

Table 1
Corn Stover Composition and elementary composition [35–38].

Component	Corn Stover [dry wt%] ^a
Glucan	33.45
Xylan	20.13
Lignin	17.22
Ash	5.40
Acetate	2.08
Protein	3.47
Extractives	13.23
Arabinan	2.69
Galactan	1.31
Mannan	0.65
Sucrose	0.37
Carbon	46.53
Oxygen	46.06

average without causing severe sustainability problems [38–40]. This lowers in average the area-specific yield.

2.2. Biochemical conversion

The basics of ethanol and biogas production are presented below.

2.2.1. Pre-treatment

To use lignocellulosic biomass as a feedstock for biogas or bioethanol production, a pre-treatment (i.e., disintegration) is necessary. The goal is to break down the non-degradable lignin and its bond with the hemicelluloses and in turn release the cellulose and hemicellulose molecules lying underneath [41,42]. The better availability of these degradable macro-molecules can reduce the retention time of the substrate within the downstream biochemical process steps and might enhance the conversion efficiency [43,44].

There are a various pre-treatment steps available based on physical, chemical, and/or biological principles (or combinations thereof) allowing to make degradable components accessible to microorganisms [45]. Due to the large number of possible applications of various pre-treatment steps, only such options are discussed here, which are either already applied on an industrial scale or show an increased technological maturity.

2.2.1.1. Hammer mill. One typical physical method of substrate digestion is a hammer mill used to enlarge the accessible surface area of the feedstock. As the absolute surface area increases with progressively smaller particles, the energy required for the hammer mill also increases clearly. With such a pre-treatment, the biodegradability of the material reduced to a few millimetres can be increased to up to 75% of the organic mass of the feedstock for various biomasses [34,43,46]. A further reduction of the biomass below the millimetre range, however, has no longer a significant influence [46].

2.2.1.2. Steam explosion. In the steam explosion process being also mainly a physical method, the feedstock is first mixed with saturated steam under elevated pressure and is held for a certain residence time before the pressure is released abruptly, resulting in an evaporation of the water present within the biomass, causing the biomass structure to crack [41]. This process can be extended with the addition of an acid / a base to further increase biodegradability [35]. Due to the high temperatures applied, degradation products can be produced that might inhibit the subsequent further decomposition of the substrate or components thereof [47]. Additionally, this process is typically very energy consuming. However, steam explosions can be used to increase the degradability towards sugars, ethanol and biogas [47–49].

2.2.1.3. Enzymatic hydrolysis. In this pre-treatment step, an

enzymatically catalysed hydrolysis of cellulose to glucose takes place. Such cellulase enzymes catalyse the reaction of water with cellulose to form shorter polysaccharides up to simple sugars [50]. This can be realized technically separately from the fermentation (SHF) or simultaneously with saccharification and co-fermentation (SCFF) [51]. In the case of a separate hydrolysis, this takes place at higher temperatures compared to the fermentation, as the enzyme activity increases with temperature up to a certain degree (i.e., faster conversion) [35].

2.2.2. Ethanol production

Ethanol is produced worldwide today mostly via biotechnological processes. Yeasts (e.g., *Saccharomyces cerevisiae*), bacteria (e.g., *Clostridium sporogenes*) or fungi can be used for this. The most commonly used ethanol production process so far is via *Saccharomyces cerevisiae* [52]. The yeast degrade glucose to ethanol and CO₂ via the Embden-Meyerhof pathway. Beside this pathway, also other conversion routes based on other yeast or bacteria strains have been identified [50, 51]. In order to generate higher ethanol yields, metabolically engineered bacteria (e.g., *Z. mobilis*) can also be used allowing to use an enhanced feedstock basis [53–55]. After fermentation, the ethanol is separated from the fermentation broth typically by distillation. If purification of the azeotropic ethanol-water-mixture is needed, an absolutisation must take place via a further process step [56,57].

2.2.3. Biogas production

During biogas production, degradation of the biomass takes place by various groups of microorganisms under strictly anaerobic conditions. Therefore, the biomass is first hydrolysed enzymatically before a CH₄ and CO₂ mixture is produced via various intermediate enzyme-catalysed steps and substances, such as acetate [58]. Biogas production is currently carried out at large scale with various feedstocks [59,60]. Mostly, a mesophilic (35 to 40 °C) mode of operation is chosen requiring less heat compared to a thermophilic fermentation (ca. 50 °C) [61]. The composition of the biogas produced varies depending on the composition of the feedstock, the retention time and lots of other influencing parameters [62]; typically roughly 50 to 55% CH₄ and 45 to 50% CO₂ can be expected. Finally, the biogas released from the substrate is purified to separate the CH₄ from the CO₂ and other gases such as H₂S [63].

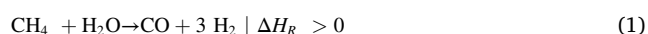
2.3. Thermochemical conversion

In addition to the processing steps presented, thermochemical conversion steps are possible, based on these biotechnologically produced intermediates. Such conversion steps are described below.

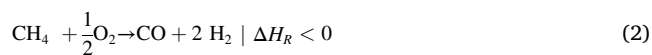
2.3.1. Reforming

Hydrocarbon reforming converts a stable hydrocarbon molecule into reactive molecules that can be used for various downstream synthesis steps (e.g., methanol, Fischer-Tropsch or mixed alcohol synthesis). This resulting gas mixture of potentially active molecules typically consists of the two gases carbon monoxide and hydrogen. The desired ratio of these two components to each other is determined by the desired downstream synthesis reaction. Depending on the demanded composition and the used feedstock, such a synthesis gas production can be carried out using different reforming technologies [64].

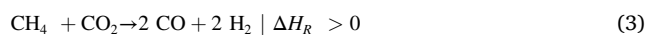
- In the steam reforming process (Eq. (1)), water and light hydrocarbons, mainly methane, are converted into a synthesis gas with a H₂/CO ratio of at least 3. This endothermic reaction requires temperatures of 800 to 1 000 °C and is usually operated at pressures of 20 to 30 bar. In order to ensure the necessary heat transfer within the reforming reactor, e.g., tube bundle reactors are used [65–67].



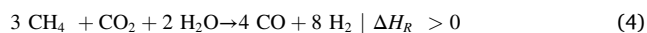
- In the partial oxidation process oxygen is added to methane to produce the synthesis gas by partial oxidation of the methane to carbon monoxide (Eq. (2)) by releasing heat (exothermic reaction). Defined by the molar ratio, a synthesis gas is produced with a H₂/CO ratio of approximately 2. Due to a subsequent reaction of carbon monoxide with oxygen, and the water gas shift reaction which might take place in parallel, in reality the H₂/CO ratio tends to be lower, ranging from 1.6 to 1.9. In order to avoid a large proportion of inert materials such as nitrogen within the synthesis gas, the oxygen must be available in a pure form within another upstream process [67,68].



- In dry reforming, CO₂ is added as an oxidant to methane. The resulting reaction takes place at a pressure level of 20 to 40 bar and temperatures of 700 to 900 °C. The stoichiometrically produced H₂/CO ratio is 1 and is therefore typically too low for the subsequent syntheses (Eq. (3)) [69,70].



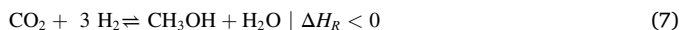
- A combination of steam reforming and dry reforming of methane (CSDRM) can be carried out to adjust the H₂/CO ratio in terms of synthesis and to use both carbon dioxide and methane as carbon sources. The H₂/CO ratio to be set depends on the ratio of the various feedstock and the respective process conditions; typically, an H₂/CO ratio of 2 can be achieved (Eq. (4)) [71]. This reaction is also strongly endothermic, like both single reactions, and requires high temperatures of over 850 °C [72,73].



2.3.2. Alcohol production

Beside the production of alcohol, such as ethanol and butanol, via the biochemical process route, alcohol can also be produced by thermochemical processes from a synthesis gas. Such a synthesis-based alcohol production is used in particular for the production of methanol, but can also be used for the production of higher alcohols via the so-called mixed alcohol synthesis (MAS).

The syngas-based methanol production is a well-known process. Methanol formation occurs either via the production of CO and subsequent methanol formation Eq. (5) and (6) or direct CO₂ hydrogenation to methanol (Eq. (7)).



According to the principle of Le Châtelier the equilibrium-limited methanol formation is favoured by low temperatures and high pressures. The operation conditions in today's low-pressure methanol synthesis are 40 to 100 bar and 200 to 300 °C. The CuO and ZnO based catalysts enable a selectivity above 99.9% while the per-pass conversion can lie close to the reaction equilibrium [29,74]. A decreasing conversion can be observed with an increasing CO₂ content within the syngas. In addition, water formation increases with the CO₂ content of the synthesis gas reducing the methanol concentration in the raw methanol.

The mixed alcohol synthesis is another possibility for synthetically producing higher alcohols. However, unlike methanol synthesis, the product mixture is not a selective compound (like methanol provided by the methanol synthesis), but a mixture of various short-chain alcohols,

including methanol. This thermochemical conversion to higher alcohols is not yet being carried out on an industrial scale, since on the one hand the competing biotechnological processes are very selective and on the other hand the currently available catalysts show comparatively low conversion rates and additionally a low selectivity with regard to higher alcohols [75,76].

2.3.3. Alcohol to jet

The general process route to obtain jet fuel from alcohol is specified in ASTM D7566. Currently, only ethanol and isobutanol are considered as feedstock for the conversion, but the goal is to widen the standard to allow all alcohols with a chain length between ethanol and pentanol (C₂ to C₅ alcohols) in the years to come. For ethanol and isobutanol, ASTM describes the four main process steps of dehydration, oligomerization, hydrogenation and fractionation. These processes are also in general applied for the conversion of alcohols into any other hydrocarbons [17, 77]. Regardless of the missing approval of the AtJ process route based on methanol by a valid ASTM standard, the basic process steps are identical [75].

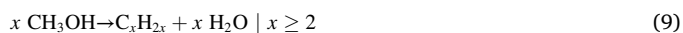
These processing steps shown schematically in Fig. 1 are described below, first in general and then specifically in regard to ethanol and methanol as a feedstock.

2.3.3.1. Dehydration. Within this first step, the hydroxy group is removed from the alcohol by forming water. In parallel, short-chain alpha-alkenes are composed. Dehydration is necessary to remove the chemically bound oxygen since no bound oxygen is allowed to be present in the subsequent end product of the kerosene fraction, according to the certification [78]. This reaction typically takes place at elevated temperatures of around 400 to 550 °C and moderate pressures of below 5 bar [79,80]. This depends, amongst other things, on the alcohol, which is dehydrated.

In the case of higher (C₂₊) alcohol dehydration, various process concepts are available. Common to all of these processes is the selective conversion of the higher alcohol molecule to the equivalent long alkene (Eq. (8)), with a limited formation of other by-products such as methane or CO₂ [80–84].



Due to the one-atom carbon derivative methanol, the dehydration of methanol does not only take place by splitting off oxygen as water, but additionally at least a carbon-carbon double bond must be achieved so that alkenes with different short chain lengths are formed (Eq. (9)). The respective process is called methanol to olefins (MtO) [79,85].



2.3.3.2. Oligomerization. Then, the alkene-rich product from dehydration is oligomerized to achieve a chain extension through the formation of carbon-carbon single bonds between the single alkenes (Eq. (10)). The starting product can be either a mixture of alkenes or a pure alkene such as ethene or butene. In both cases, a product mixture of alkenes of different chain lengths is obtained. [78,86,87]. This oligomerization step is typically controlled by catalysts and takes place at moderate temperatures of 100 to 250 °C and elevated pressures of >20 bar [88, 89].



During oligomerization, mainly even-numbered multiples of the alkenes are produced since one additional ethene molecule is bonded to each growing chain. Only to a limited extend longer alkene chains might break and thus produce non multiples of the alkene hydrocarbon chain length [78,89]. If oligomerisation is initiated from an alkene mixture, as is the case after methanol dehydration, the product tends to be a more diverse mixture compared to an oligomerization of alkenes from higher alcohols. Such an oligomerisation of an alkene mixture from the MtO

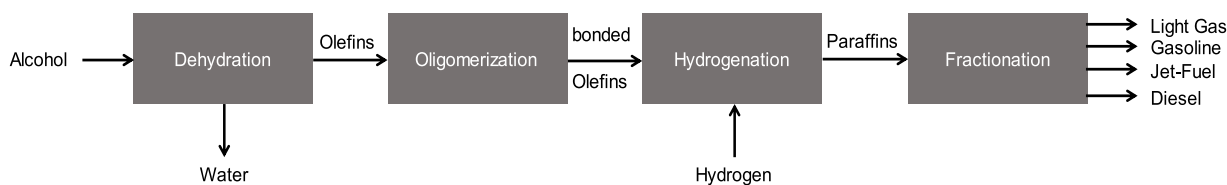


Fig. 1. Main alcohol to jet process steps.

technology is realized on an industrial scale to obtain fuels such as gasoline from methanol [90].

2.3.3.3. Hydrogenation. Now hydrogen is added to saturate the remaining double bonds and thus to produce alkanes. This can react with a noble catalyst such as platinum even at a slight overpressure of less than 10 bar and at ambient temperature. Technically, more cost-efficient catalysts are usually used and higher temperatures and pressures are applied. [91]. The required amount of hydrogen corresponds to the molar amount of alkenes to be saturated (Eq. (11)) [92]. This hydrogen can be supplied via different routes. Since the production of a SAF requires a hydrogen supply characterized by low greenhouse gas (GHG) emissions, the production of hydrogen via electrolysis using electricity from renewable sources of energy seems to be a promising option.



2.3.3.4. Fractionation. In the final step, the hydrocarbon mixture is divided into different product fractions according to their chain length to fulfil the given fuel standards e.g., for the Jet-Fuel fraction (i.e., to maintain the boiling curve specified within the respective ASTM standard) [17].

3. Methodology

The processes to be analysed are first designed on the basis of the overarching framework requirements and then analysed with each other using the simulation approach with the help of technical parameters.

3.1. Process design

In order to make the processes comparable with each other, the framework assumptions of the process chains must be identical. The basic feedstock for all processes is corn stover. These processes are designed for a constant kerosene production volume. Furthermore, the process is provided with as much heat energy and electricity as it requires. An interconnected process will be designed, which will then be used to interconnect the various material and heat flows.

Within these system boundaries, technologies for the individual process steps are selected with the goal to ensure a high degree of technical readiness, a high carbon efficiency and synergies with each other. Large scale electrolysis for the provision of hydrogen to reduce possible carbon losses in form of CO₂ is not considered, as the processes focus on fuels primarily from biogenic sources. The limited demand for pure hydrogen needed for upgrading the products is nevertheless covered by electrolysis, as this avoids the separation of hydrogen from the synthesis gas. The process designs are essentially determined based on individual process data and it is assumed that they can be interconnected to form an overall integrated process. Since feedstock and product logistics are similar for all processes considered here, they are not considered in detail.

3.2. Simulation approach

The technical analysis of jet-fuel production processes described above is carried out based on steady-state flowsheet simulations. The

previously designed processes are converted into a steady state flow-sheet simulation model. Building on the model results from the stationary flowsheet simulation, the mass, material and energy balances are determined and closed. A pinch analysis is performed for analysis of the energy balance, while identifying the external cooling and heating requirements and carrying out an ideal heat integration. This simulation approach is carried out with the simulation program Aspen Plus®.

3.3. Technical analysis

For the technical comparison of the various production processes, material- and energy-related indicators are defined. The theoretical carbon efficiency and the bio-chemically possible carbon efficiency are determined as two material-related indicators. Additionally, the energetic efficiency is used as an energy-related indicator. Based on these three indicators, the processes are later compared with each other.

Eq. (12) defines the theoretical carbon efficiency of a process or process chain. This carbon efficiency can be related both to the target product kerosene ($\eta_{C,Kero}$) or to all valuable carbon-containing energy carrier / products ($\eta_{C,HC}$) in case those side-products should also be taken into account.

$$\eta_{C,theo,Prod} = \frac{\dot{n}_{C,Prod}}{\dot{n}_{C,F}} \quad (12)$$

$\eta_{C,theo,Prod}$ Theoretical carbon efficiency for product fraction

$\dot{n}_{C,F}$ Carbon molar flow in feedstock

$\dot{n}_{C,P}$ Carbon molar flow in considered product

In addition to the theoretical carbon efficiency, a bio-chemical carbon efficiency is analysed. Here it is assumed that all heteroatoms that cannot be used for the respective end product must leave the process in their highest oxidation state (Oxidation state oxygen: - II). If this were not the case, an external energy requirement (i.e., electrolysis) would be necessary to reduce the oxygen, although this external energy requirement is not considered in this study.

During the conversion of biomass-based macro molecules (e.g., cellulose) into chemical compounds (i.e., hydrocarbons within the kerosene blend) with clearly defined characteristics, the biogenic raw material (feedstock) usually lacks hydrogen and has a surplus of (unwanted) oxygen. Both deviations from the ideal ratio can be overcome by separating CO₂ from the biogenic feedstock; but such an approach shows the clear disadvantage that the carbon availability for the overall process is reduced (the carbon contained within the CO₂ is considered to be a loss). In addition, depending on the extent of each of these deviations, the oxygen content of the organic macromolecules can also be circumvented by the formation of water (with the consequence of a hydrogen loss); conversely, the hydrogen deficit can be reduced by the addition of water. The carbon remaining after this compensation can be assessed by the bio-chemical carbon efficiency. With this indicator, the efficiency of the biochemical conversion can be expressed, while taking into account the dependency on the feedstock composition.

To determine this, the molar ratios of the target product are first defined in Eq. (13) and 14.

$$X_{H:C} = \frac{\dot{n}_{H,chem}}{\dot{n}_{C,chem}} \quad (13)$$

$$X_{O:C} = \frac{\dot{n}_{O,chem}}{\dot{n}_{C,chem}} \quad (14)$$

- $X_{H:C}$ Hydrogen to carbon ratio in the target product
 $X_{O:C}$ Oxygen to carbon ratio in the target product
 $\dot{n}_{H,chem}$ Biochemically possible hydrogen flow in the target product
 $\dot{n}_{C,chem}$ Biochemically possible carbon flow in the target product
 $\dot{n}_{O,chem}$ Biochemically possible oxygen flow in the target product

Using these target ratios of the products and the molar composition of the feedstock, the remaining chemical carbon flow of the feedstock can be calculated based on Eq. (15). The carbon flow achieved in the provided product can then be assessed on this carbon flow in order to calculate the chemical carbon potential (Eq. (16)).

$$\dot{n}_{C,chem} = \frac{\dot{n}_{O,F} - 2 \dot{n}_{S,F} - 2 \dot{n}_{N,F} - 2 \dot{n}_{C,F} - \dot{n}_{H,F}}{X_{O:C} - 2 - X_{H:C}} \quad (15)$$

$$\eta_{C,chem} = \frac{\dot{n}_{C,Prod}}{\dot{n}_{C,chem}} \quad (16)$$

- $\dot{n}_{O,F}$ Oxygen molar flow in feedstock
 $\dot{n}_{S,F}$ Sulfur molar flow in feedstock
 $\dot{n}_{N,F}$ Nitrogen molar flow in feedstock
 $\dot{n}_{H,F}$ Hydrogen molar flow in feedstock
 $\eta_{C,chem}$ Bio-chemical carbon efficiency for product fraction

Equivalent to the carbon balance, an energetic efficiency is also defined (Eq. (17)). In addition to the energy input of the material flows calculated based on the higher heating value (HHV) the energy input in the form of heat and electricity is also included.

$$\eta_{e, Prod} = \frac{\dot{m}_{Prod} HHV_{Prod}}{\dot{m}_F LHV_F + P_{el} + \dot{Q}} \quad (17)$$

- $\eta_{e, Prod}$ Energy efficiency for product fraction
 \dot{m} Mass flow
 HHV_{Prod} Higher heating value
 P_{el} External electricity demand
 \dot{Q} External heat demand

4. Conceptual design and data assumption

Based on the procedure described, the framework assumptions for all processes are described below, before the individual process assumptions are presented.

4.1. Framework assumptions

Based on the state of the art presented in chapter 2, processes are designed in this section for a targeted kerosene production of 1 t h^{-1} . The heat to be provided depending on the process configuration is provided at four different temperature levels (125 °C; 175 °C; 250 °C; 1 000 °C). These correspond to different water vapour pressures and a high temperature source. The electricity to be provided by renewable sources of energy in order to reduce the GHG emissions of the process chain. All processes use corn stover as feedstock. This lignocellulosic biomass is widely available and is currently only used to a limited extent. A moisture content of 20% and a size of corn stover material of 20 mm are assumed. The processes are designed in such a way that other feedstock compositions can also be investigated, since the results depend, amongst other things, on the structural composition of the

feedstock.

4.2. Ethanol to kerosene pathway

In the ethanol-based process route, the corn stover is first treated with steam inside a steam explosion process by using additionally $18 \text{ mg}_{\text{dry}}^{-1} \text{ H}_2\text{SO}_4$. Prior to that, no further reduction of corn stover material is assumed. After this treatment the vapour phase is separated from the liquid phase; the latter is then moved directly to the fermentation as a first liquid phase. The remaining solids characterized by a high water content are fed together with enzymes into the enzymatic hydrolysis for further breakdown of the biogenic macromolecules. The product of the respective hydrolysis is then separated into a solid and a liquid phase within a decanter. The solid phase mainly consisting of lignin can either be used as a by-product and returned to the field or dried further for burning / energy provision.

For this, two different process concepts “EtJ” (Ethanol-to-Jet) for the process concept without combustion of the solid phase and “EtJ-Burn” (Ethanol-to-Jet with lignin burning) to consider combustion are defined.

The first liquid phase coming directly from the steam explosion and the liquid from the decanter are fed into the fermenter, where alcohol production realized by *Z. mobilis* takes place. Next, the resulting fermentation broth is purified by distillation to 92 wt.-% ethanol purity (i.e., just below the azeotropic point of the mixture). Such a high degree of purification reduces the efforts for the subsequent dehydration. Because a water-ethylene separation is required anyway after the dehydration step, this concept does not include an absolutisation process.

Dehydration subsequently takes place within the gas phase. The resulting gas mixture is first separated from the water by distillation and then the CO_2 is eliminated in a caustic wash and further H_2O impurities are removed with a molecular sieve. These components might inhibit the next process step of oligomerisation [89]. In this reaction step, the alkenes are converted to alkenes meeting mainly in the required chain length distribution of kerosene. The resulting mixture of long-chain alkenes are then separated and mixed with hydrogen within a hydrogenation process. “Green” hydrogen from electrolysis is assumed to be used for this treatment step. In the final fractionation step, the alkanes are separated into different fuel fractions. Here, all hydrocarbons with a chain length between 9 and 16 carbon atoms are classified as part of the kerosene fraction. In the gasoline fraction, hydrocarbons with a chain length between 5 and 8 carbon atoms are included and in the diesel fraction, chain lengths with more than 16 hydrocarbon atoms are allocated. Lighter fractions than the gasoline fraction are separated as light gas.

The described process concept is shown in Fig. 2. In addition to the main products, the fuels, various by-product streams such as flue gas, waste water, CO_2 and O_2 are also produced. CO_2 and O_2 might have an economic value, but do not directly influence the energy balance. Additional information about the detailed process settings are given in supplementary material appendix A.

4.3. Biogas to kerosene pathway

In the biogas to kerosene pathway, the corn stover is first shredded within a hammer mill [94]. The shredded corn stover is then fed directly into the anaerobic digestion system producing biogas and the remaining digestate. The latter can either be returned to the field (GtJ) or, after a further drying step, used for direct energy production within the process chain (GtJ-Burn).

The biogas is then purified by first adsorbing hydrogen sulphide and then separating the CO_2 with the help of a membrane process. The aim is to achieve a molar ratio of 1 to 3 for the CO_2 to CH_4 ratio. In the subsequent combined dry and steam reformer (CDSRM), this leads together with water to a targeted synthesis gas ratio of approximately 2 to 1 for H_2 to CO required for the subsequent methanol synthesis. Thus,

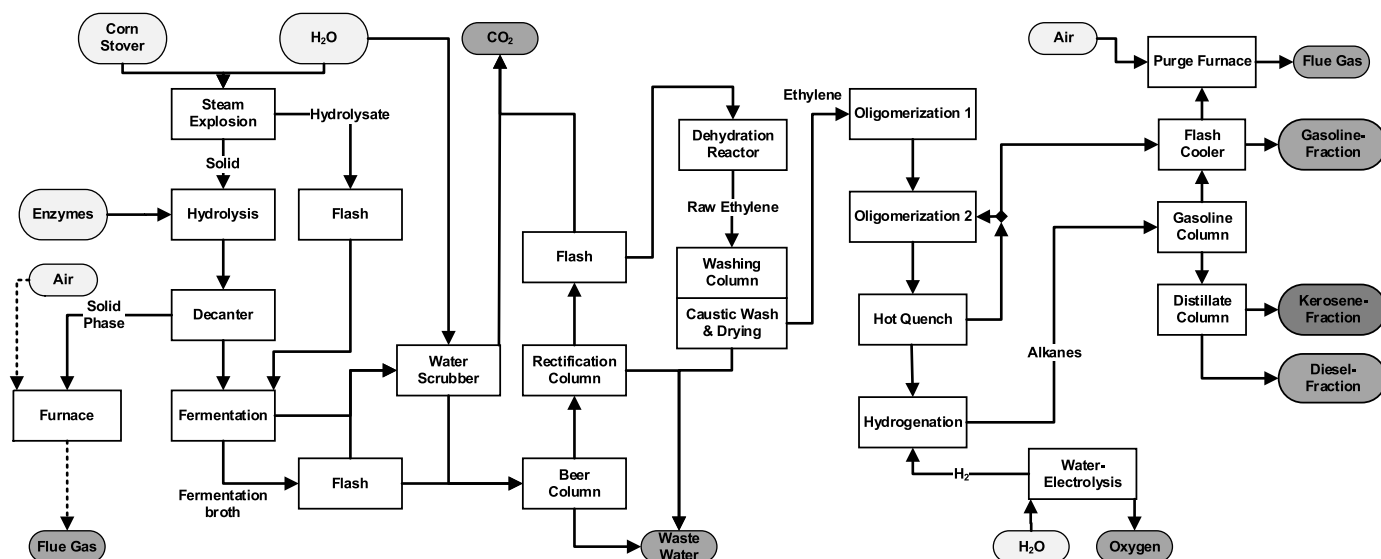


Fig. 2. Conceptual design biomass via ethanol to jet fuel (Dotted streams and processes only included in case of burning | Detailed process description is shown in supplementary material appendix A and is based on e.g. [35,80,89,93]).

methanol synthesis is assumed to start from CO-based synthesis gas.

After the methanol synthesis step, the unreacted gas is first recycled and the water is separated by distillation. The crude methanol is then dehydrated in a MtO plant to a mixture of short-chain alkenes. These are then also separated from the by-product water; remaining CO₂ is removed within a caustic wash. This alkene mixture undergoes then the oligomerisation process step. For that, a generic oligomerisation according to an adjusted Anderson Schulz Flory (ASF) distribution is assumed. The alkenes, which are too short-chained, are separated and recycled. The longer alkenes are added to a hydrogenation reactor together with hydrogen from water electrolysis to hydrogenate the alkenes to alkanes. Finally, the different fuel fractions produced in the oligomerisation are also separated within several rectification columns. The same fraction splitting is aimed for as in the ethanol-based process route.

The entire process is shown in a block flow diagram in Fig. 3. The by-products water, flue gas and potentially the digestate are also shown

next to the main products. In addition, CO₂ and oxygen are also produced in pure form. Detailed information on the basic assumptions of the individual process steps for the process pathway are documented in supplementary material appendix B.

5. Results and discussion

In this chapter, the results are first outlined and then discussed for each individual process before they are compared with each other. The sankey diagrams presented in this chapter are for all streams relative to the input stream of the corresponding parameter (carbon or energy) into the overall process. The composition of the product streams from the process simulation are shown in more detail in appendix C.

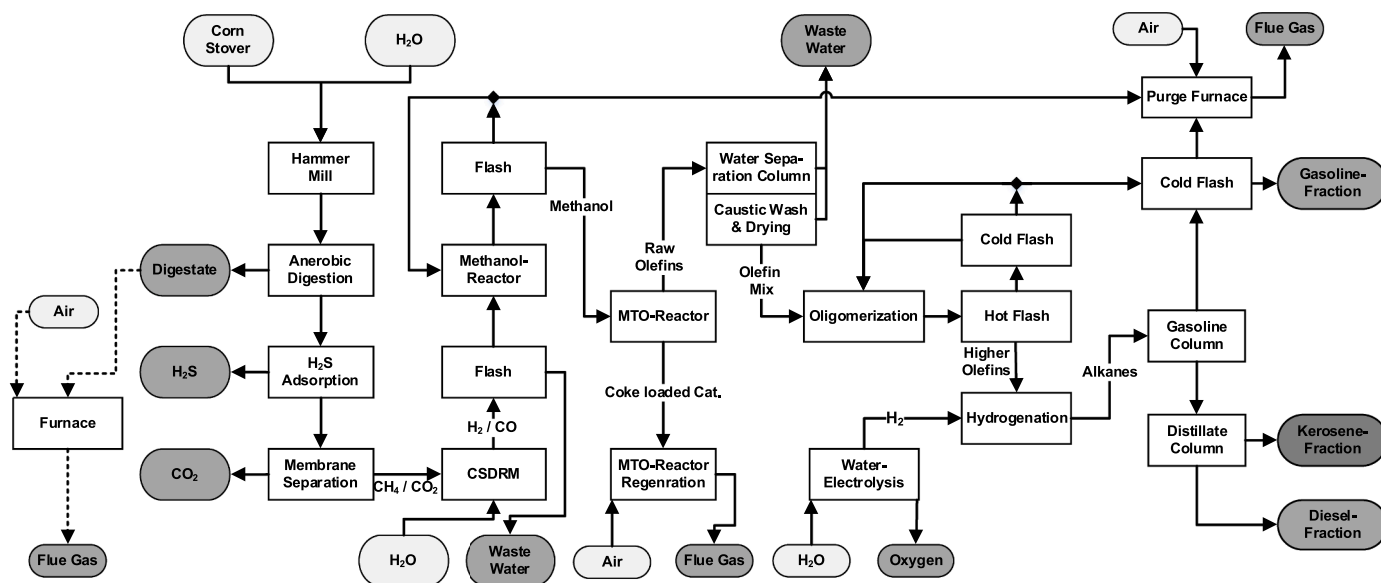


Fig. 3. Conceptual design biogas to kerosene pathway (dotted streams and processes only included in case of burning | Detailed process description is shown in supplementary material appendix B and is based on [33,34,73,95–97]).

5.1. Ethanol pathway

Results

The simulation results of the EtJ process routes for the carbon and energy flows are presented below.

Carbon flow. Fig. 4 shows the theoretical carbon balance. Thus, the main carbon input into the overall process is with more than 99% the primary feedstock corn stover. In addition, a small amount of carbon is added to the system by the required enzymes (0.7%). But already within the pre-treatment of the corn stover, 34.1% of the carbon is removed from the process in form of mainly lignin; this carbon respectively the corresponding energy can still be used for heat generation in the case of combustion.

During and after fermentation, carbon is also “lost” as CO₂ and biomass unconverted into ethanol. During further processing of ethanol into hydrocarbons, only minor carbon losses occur. Here, 3.3% of the carbon is discharged within the oligomerisation cycle to prevent an accumulation of inerts within the synthesis cycle.

All in all, a theoretical carbon efficiency of 23.4% can be achieved with regard to the kerosene fraction. Related to all valuable hydrocarbon fractions, an overall carbon efficiency of 28.1% is possible.

Energy flow. The energy flow for the case without the combustion of the solid, pre-treated biomass are shown in Fig. 5 and the case with the combustion of the biomass are depicted in Fig. 6. Thereby, sometimes more than one stream is combined in the individual blocks to simplify the energy flow. In addition, the heat balance cannot be closed in every single process shown, because the material flows have different heating values and also different temperatures between the steps.

If the remaining unusable solid biomass components are not burnt, 80% of the total energy input into the process is provided by the corn stover itself. In addition, there is an energetic input of 17.7% required in form of heat. The remaining energy input into the process is electrical energy required at various points, such as for compressors or for electrolysis for hydrogen provision for saturating the alkenes. For the pre-treatment step steam explosion, 63.2% of the total energy input is already required in form of thermal energy to evaporate the water. However, to a limited extent heat can be recovered there.

In addition, thermal energy being 14.2% of the overall input energy is required to purify the ethanol after the fermentation step. As with the carbon balance, the subsequent thermochemical conversion of ethanol to hydrocarbons does not require an absolute larger energy contribution. After these conversion steps, a total of 28% of the overall energy can be recovered in form of kerosene and 33.5% as hydrocarbons.

If the solid residues are used to generate heat in a process furnace, the external heat demand is reduced to 0%. In addition, 3.6% of the total

energy can be used to produce steam (Fig. 6). With this process step, the overall efficiency of the process can be increased to 34% with regard to paraffin and to 40.8% with regard to total hydrocarbons.

Discussion

Below the results outlined above are discussed and interpreted.

Carbon flow. In addition to the target intermediate ethanol, the fermentation step also produces a pure CO₂ waste gas stream. Although this is not considered so far as a value product for biogenic processes, it can serve as a sustainable carbon source for power-based synthesis production processes. The two-step oligomerization simulated in this model shows a high carbon selectivity towards the kerosene fraction. This can be explained by the different reaction conditions of the two oligomerization reactors. In the first oligomerization reactor, mainly ethene is oligomerized to C₄ to C₈ alkenes before this is subsequently fed to the second reactor. Due to these reactor concept, a selective oligomerization towards the kerosene fraction can be achieved.

Energy flow. According to these diagrams, a large amount of energy is already required to make the carbon available for the ethanol fermentation and the subsequent ethanol purification. Although this can be partly covered by internal heat generation, it must be supplemented with the provision of medium-pressure steam. Only in the case of combustion of solid residues no additional heat from external sources is required. The pre-treatment step therefore has a decisive influence on the efficiency of the entire process chain.

The thermochemical process steps show lower carbon losses and energy consumption compared to the previous biochemical process steps and its purification steps. This is because these processes already have a lower total throughput than the upstream processes, due to a much lower water content in the processing stream, which is why the heating and cooling of water in the quantities is no longer necessary. With over 80% carbon and energy efficiency from ethanol to kerosene, the thermochemical processes are efficient. This is partly due to the fact that the processes are focused on a specific feedstock and not, as in the fermentation step, on a mixture of different classes of substances in the feed.

5.2. Biogas pathway

Results

The simulation results of the EtJ process routes for the carbon and energy flows are presented below.

Carbon flow. The theoretical carbon balance of the GtJ and GtJ burn case is shown in Fig. 7. Following this, the complete carbon inventory of

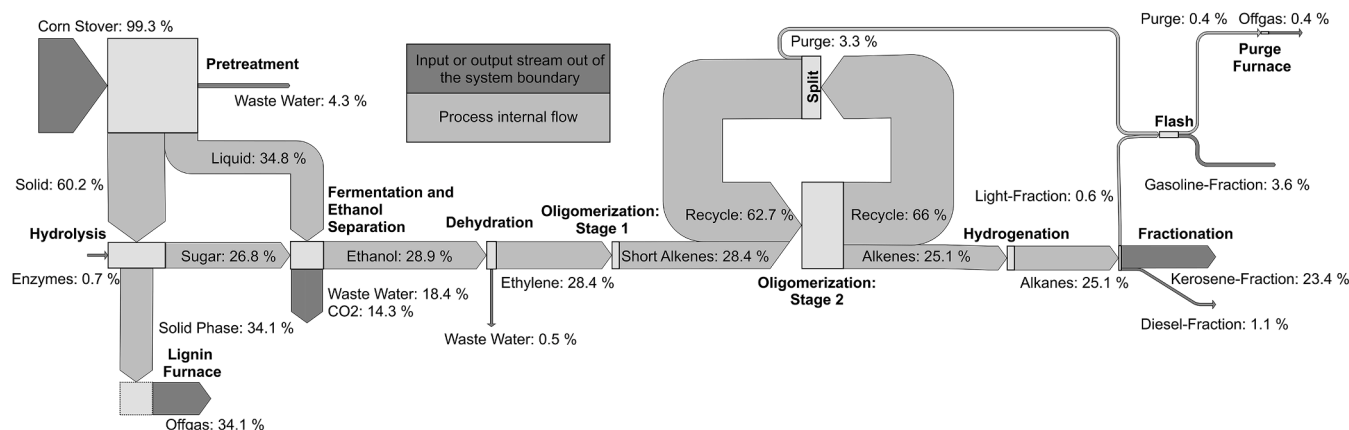


Fig. 4. Theoretical carbon efficiency for the ethanol pathway.

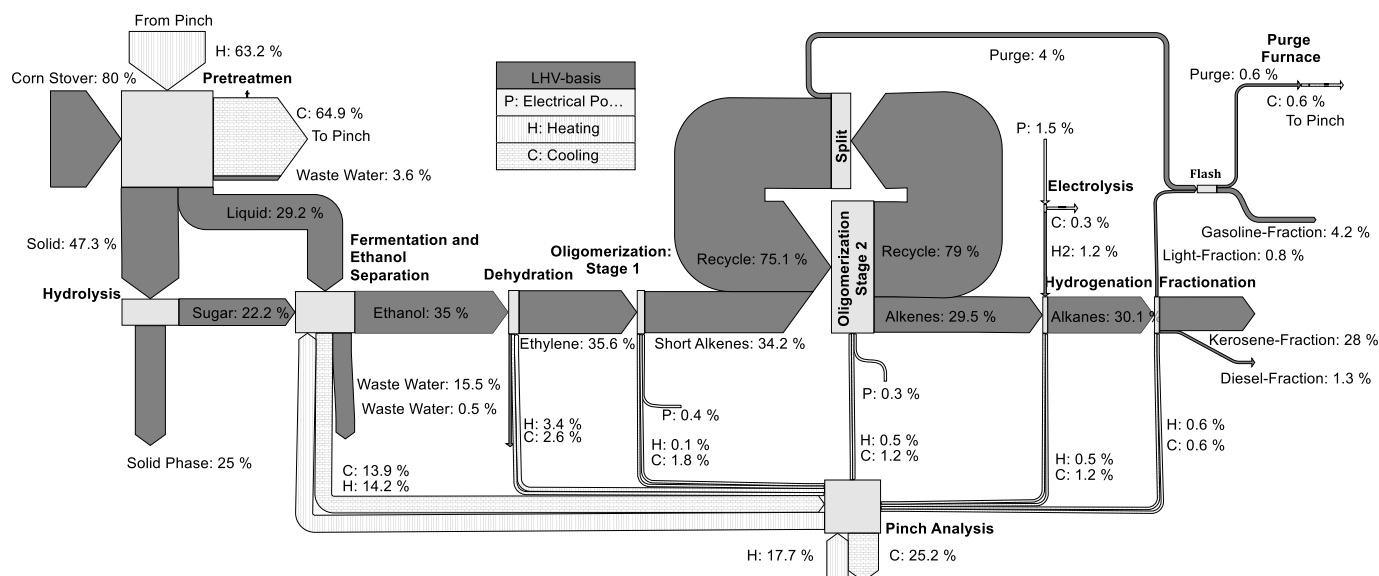


Fig. 5. Energy efficiency for the ethanol pathway without solid combustion.

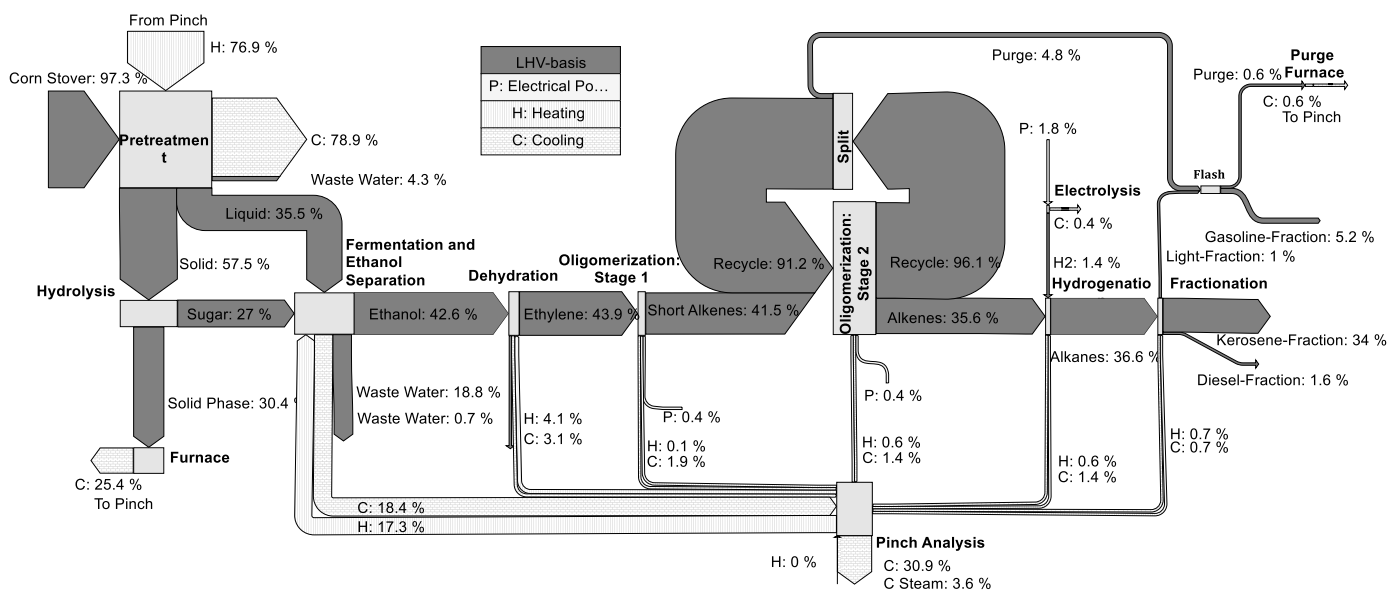


Fig. 6. Energy efficiency for the ethanol pathway with solid combustion.

the organic feedstock is fed into the biogenic reactor. In addition to the main product biogas (a CO_2 and CH_4 mixture), digestate is produced as a by-product to be dried before the optional combustion. Typically, 44.1% of the carbon contained within the corn stover is found in the biogas. As this also consists roughly half of CO_2 , a part of this must be separated to achieve the correct CH_4 and CO_2 ratio for the subsequent reforming. After the following methanol synthesis, about 31.9% of the carbon input can be found in the provided methanol. This methanol is then converted to long chain hydrocarbons. After this process, a total of 18.9% of the carbon can be found within the kerosene fraction. The carbon losses appear due to a broader oligomerization distribution since only one oligomerization step was chosen here, and due to the short chain alkane and CO_2 by-products of the MTO plant assumed to be a loss related to the main product.

Energy flow. The energy balance of the GtJ process route is shown in Fig. 8. The combustion and the associated energetic use of the digestate can be seen in Fig. 9. In the case of non-energy use of the digestate,

85.5% of the input energy is fed into the process in the form of corn stover, with an additional 6.1% of the energy being fed into the process in the form of external heat and 8.4% by electricity. 42.1% of the energy used – based on the energy content of the reactants – is obtained in the form of biogas. This biogas is converted into synthesis gas in the combined steam and dry reformer, which in turn has a high external heating requirement at temperatures of 1000 °C. This external heating is not required if the digestate can be used (burnt) as a source for high-temperature production. In both cases, excess heat is produced throughout the process chain, which is brought out of the system boundary in the form of potentially valuable steam. In the case of non-combustion of the digestate, this heat cannot be used within the process, as the additional heat required is needed at a higher temperature level, and cannot be provided by steam. Due to the slightly over-stoichiometric syngas ratio in the make-up gas, large energetic recycles are required within the synthesis loop, as there is a high hydrogen content in the loop. However, the amount of purge to be removed is low at 1.3% overall, but strongly depends on the assumed purity of the biogas. All in all, in the

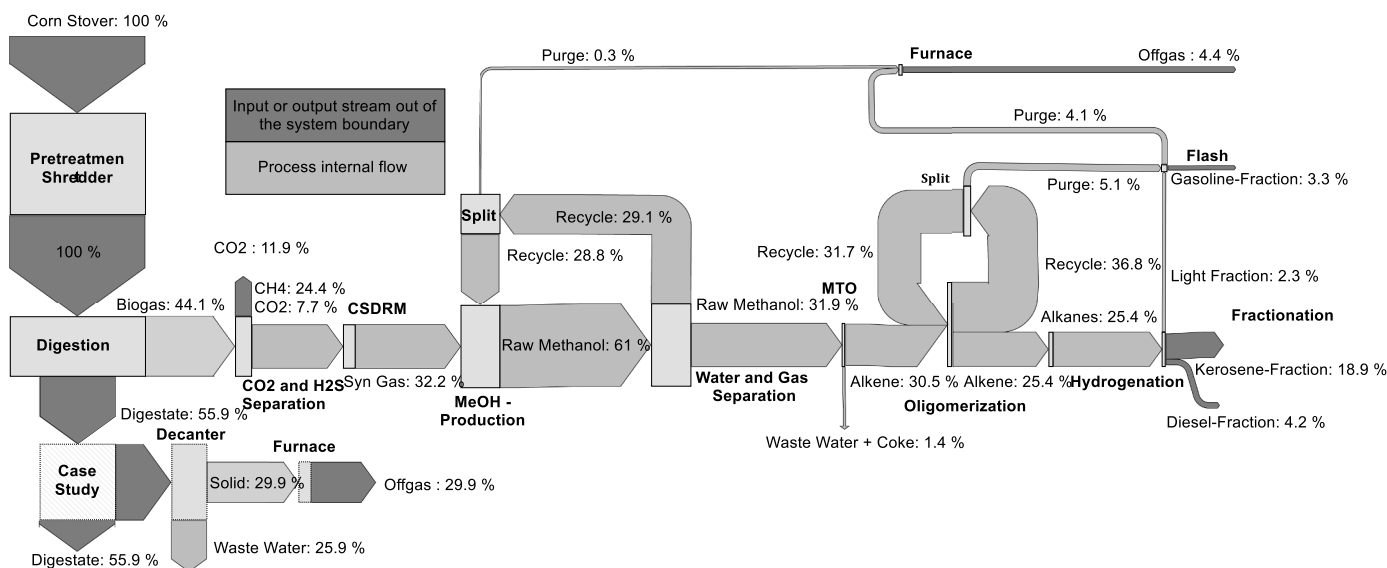


Fig. 7. Theoretical carbon efficiency for the biogas pathway.

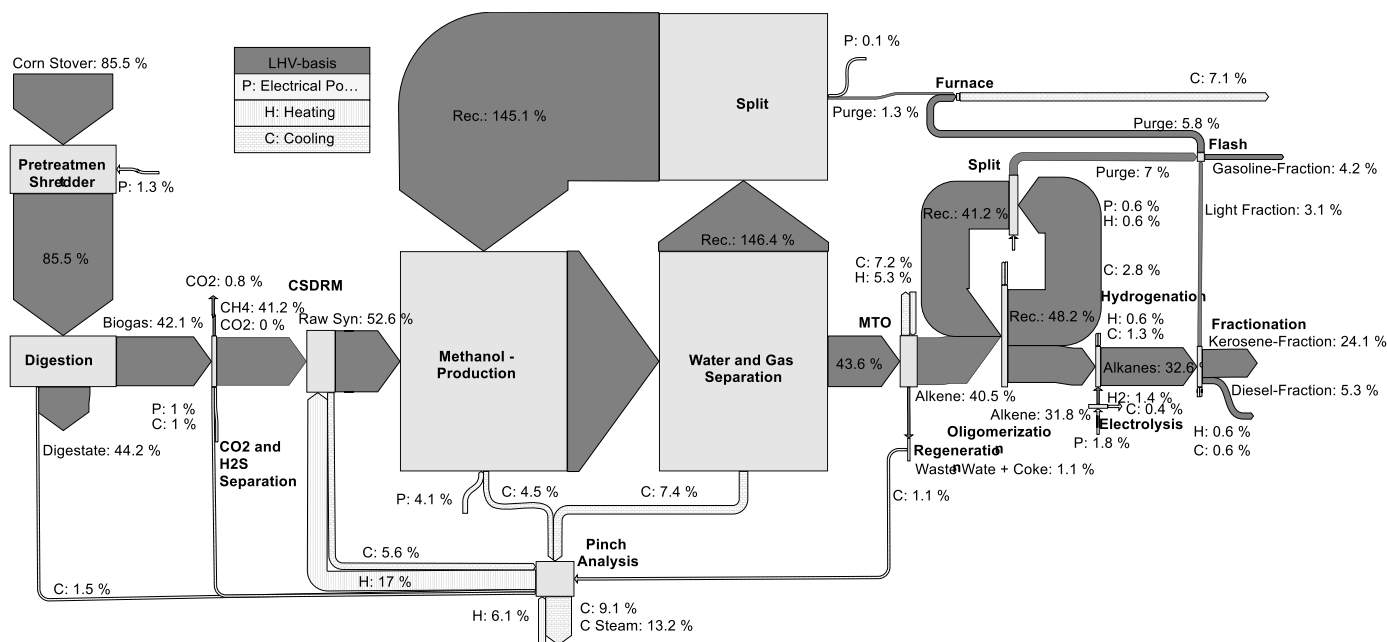


Fig. 8. Energy Efficiency without Solid Combustion for the Biogas Pathway.

GtJ case an energy efficiency with respect to kerosene of 24.1% can be achieved.

In the case of the combustion of digestate, this efficiency can be increased to 25.7%. This small increase in energy efficiency can be explained by the low external heat demand and the resulting lower substitution. However, a larger amount of steam can be produced. In addition, a total of 35.8% of the total energy input is generated as hydrocarbon end products.

Discussion

Below the results outlined above are discussed.

Carbon flow. The shredding of the corn stover as pre-treatment measure results in no carbon losses and only low energy requirements. Thus, all biomass enters the core biochemical conversion step maximising potential carbon conversion. Since the CO₂ to CH₄ ratio of raw biogas is too

high to produce a molecular suitable synthesis gas, CO₂ is separated. This causes carbon losses, but at least no major energy losses. Reducing CO₂ using CH₄ and water requires external heat but improves the carbon yield for the whole process.

Energy flow. Due to the moderate to high stoichiometric number synthesis gas in the make-up gas of the synthesis cycle, the hydrogen in particular is concentrated in the recycle and thus increases the stoichiometric number of the synthesis gas. As a result, the energy-based recycle is high, while the carbon-based recycle remains lower. In addition, the recycle is increased by adding inert substances such as nitrogen. Nitrogen is present in small amounts in the biogas and was not purified in the previous gas purification step. This nitrogen content of 2% in the biogas must be removed within the synthesis cycle in order to avoid its ongoing concentration. As a result, the corresponding proportions of hydrogen and carbon are also transferred to the purge stream.

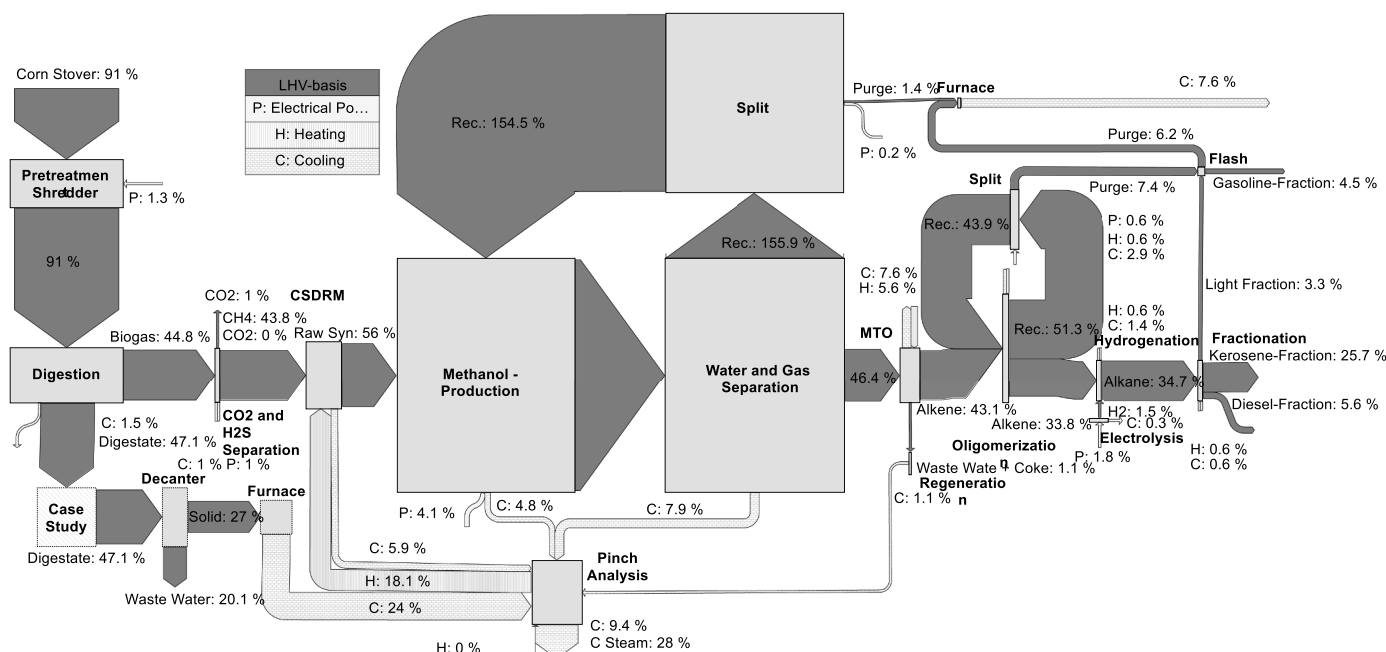


Fig. 9. Energy Efficiency with Solid Combustion for the Biogas Pathway.

Within the oligomerization of the alkene mixture of the MTO plant, both an increased energetic and carbon bound recycle is set. This is required to return the short-chain hydrocarbons to the oligomerization and allow them to react further. In addition to the kerosene, larger quantities of diesel and naphtha fractions are also produced. These fractions can also be used for the defossilization of the road transport or – especially in the case of naphtha – as a raw material for the chemical sector. This also applies to the production of steam as a by-product, which can be used in several sectors to substitute fossil fuel-based heat supply. However, it can be expected that steam production and consumption depend on time and location, with hydrocarbon energy sources being more flexible in use.

5.3. Comparison

In this section, the two processes are compared with each other in terms of carbon and energy efficiencies. First, the efficiencies with regard to the biobased intermediates (i.e., ethanol and biomethane) and the alcohol intermediate (i.e., ethanol and methanol) are presented. In the EtJ process route, the efficiencies for the biobased intermediate and alcohol are the same, since no further conversion step is necessary. With regard to the end products, a distinction is made between the target product kerosene and all valuable end products. In addition to kerosene, this includes the gasoline and diesel fractions, as well as steam, which has no influence on the carbon balance, but on the energy balance of the process chain.

Carbon flow

Fig. 10 shows the theoretical and bio-chemical carbon efficiencies. The theoretical carbon efficiencies can also be directly visualised in the sankey diagrams shown above. It can be seen that for the biobased intermediates, the carbon balance in terms of the bio-chemical carbon efficiency is only around 50% (46.1% in EtJ and 52.1% in GtJ). This is due to two decisive influencing factors. Firstly, lignin in particular cannot be degraded in the two biological processes and thus reduces the carbon yield, since in the feedstock, lignin also provides a total carbon input of around 24%. Secondly, there is the carbon, which is either not converted due to the residence time or is converted to other by-products such as biomass.

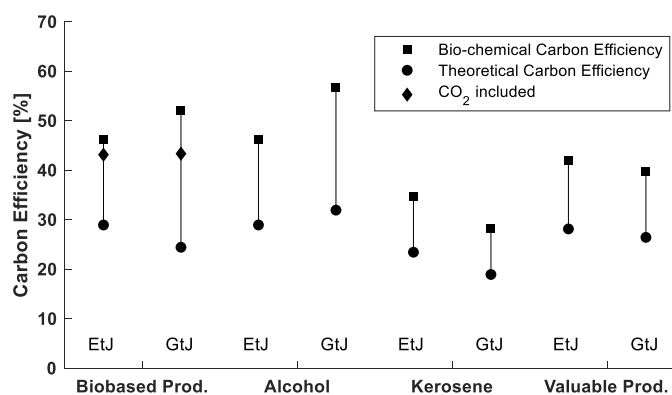


Fig. 10. Theoretical and bio-chemical carbon efficiency for both process pathways (EtJ: Ethanol to jet; GtJ: Biogas to jet).

Both biogenic intermediates must have a higher hydrogen to carbon ratio compared to the final product kerosene. Biomethane requires an H:C ratio of 4 and ethanol of 3. The feedstock analysed here has both a hydrogen deficit and an oxygen surplus. For the end product kerosene, the oxygen surplus is the decisive criterion for the bio-chemical carbon balance, but for the biogenic intermediates the hydrogen deficit is also decisive. Therefore, water must be added to the system to add the hydrogen. This in turn requires the removal of the oxygen in the form of CO₂, which in turn reduces the bio-chemical carbon potential with respect to these intermediates. Since the final product kerosene only requires a lower H:C ratio – which increases the bio-chemical carbon potential within the feedstock (cf. Eq. (15)) – the bio-chemical carbon efficiency in EtJ drops to 34.7% and in GtJ to 28.2%. In addition to the previous reasons, this drop is also related to the fact that the subsequent process steps towards kerosene analysed here require the separation of oxygen by water (Dehydration). This is therefore not ideal for utilising the bio-chemical carbon potential, as more carbon has to be indirectly separated to maintain the H:C ratio. This influence is more relevant in the GtJ case, since a higher H:C ratio is required in the biomethane and additionally a higher O:C ratio is present in the methanol. In relation to all valuable by-products, the bio-chemical carbon efficiencies increase

once again to 42.0% in the EtJ and 39.7% in the GtJ case.

In the biogenic process steps, the biogenic CO₂ can be considered as a potentially interesting product, besides the main products ethanol and methane. Within the GtJ process, CO₂ is already partially used within the process. These are added to the respective biogenic product and shown in Fig. 10. Thus, the theoretical carbon balances with CO₂ included are 43.1% in EtJ and 43.3% in GtJ.

Energy flow

Fig. 11 shows the energy efficiencies for the EtJ and GtJ and their combustion cases. In all cases, the energy efficiency in the solid combustion case is higher than in the non-combustion case. This is due to the fact that the heat produced in both cases completely eliminates the external heat demand (cf. Fig. 6 and Fig. 9), which reduces the total energy used and thus increases the energy efficiency. This effect is stronger in the case of the EtJ process, as in the GtJ case a higher external heat demand is needed.

The GtJ process route shows a higher energetic efficiency with regard to the biogenic intermediate products. Due to the heat energy input in the RWGS and the associated utilisation of a partial CO₂ stream, the energy efficiency can be increased from 39.5% for biomethane to 40.8% for methanol in the case of the non-combustion case.

In both process routes, an increased spread of efficiencies can be seen in the two cases considered when all valuable products are considered. This results from the heat production, which was represented in the model in the form of steam provision. Especially in the GtJ case, much of the combustion heat is used for steam production. Unlike hydrocarbon energy sources, heat energy in the form of steam can be transferred, but not without considering local conditions. Depending on these, heat must be used locally; if this is not possible, only a partial combustion of the remaining solid biomass could be considered as a substitute for external heat supply. If there is a direct heat consumer at the production site, this can be beneficial for the overall efficiency of the process considered here.

6. Conclusion

An inevitable step towards making the aviation industry carbon-neutral is to provide the energy source to be used in aircrafts in a renewable way. For this purpose, biogenic or non-biogenic sustainable aviation fuels (SAFs) can be used, which are similar to kerosene and can thus be feed into the current aircraft fleet and make a direct, timely contribution to carbon-neutral aviation. Today, for example, various biogenic intermediate and end products are already available that would be suitable for the production of SAFs. Unlike biodiesel, biogas and bioethanol can be obtained from a broad variety of different organic material streams containing sugar, starch or lignocellulose. The latter option offers a high material potential as well as no direct competition

with the food and feed market.

Against this background, two biogenic process pathways are compared based on a bio-chemical conversion of lignocellulosic biomass for the production of intermediate products currently available on the market; this allows for a decoupling of the process steps from each other. On the one hand this can lead to a more flexible product and process development and on the other hand it can lead to a broader availability of raw materials for the intermediate product. The goal is to compare the process routes based on biogas and bioethanol and to evaluate which process routes are more efficient with the available feedstocks and process energies on the basis of technical key figures such as carbon efficiency and energy efficiency. This analysis of carbon efficiency is performed with respect to the theoretical carbon balance as well as with the help of the bio-chemical carbon balance. The latter describes the proportion of carbon that can be transferred from a chemical atomic view into the intermediate or end product without adding additional hydrogen to the system and thus increasing the carbon yield. From an energetic perspective, a scenario realizing the combustion of the remaining solids (mainly lignin) and a scenario without such a solid biomass use are investigated. Consistent with this objective and the study methodologies, the following main results were produced:

- In the ethanol-based process route, the largest carbon and energetic losses occur during the bio-chemical conversion, despite the fact that an intensified pre-treatment was undertaken. In total, around 29% of the carbon could be transferred as ethanol, of which around 80% can be found in the kerosene end product. This indicates a high efficiency of the alcohol to jet process examined there. In terms of energy, in addition to the feed, 17.7% of the total energy input also has to be given to the system in the form of heat. All in all, if the remaining solid biomass is not burnt, 28% of the energy used is recovered in the form of kerosene.
- In the biogas-based process route, a total of 32.2% of the carbon can be used in the synthesis gas can for further processing. Of this carbon, about 59% ends up in the SAF fraction. This is partly due to the fact that the dehydration is not as selective as the ethanol dehydration and that a one-step generic oligomerization was used producing a broader product spectrum. 24.1% of the energy input can be obtained as kerosene. In addition, external heating is also required here, since the reforming step in particular, has an increased energy requirement.
- Comparing the process chains with each other, the biogas pathway has a higher bio-chemical carbon efficiency, especially towards the biogenic intermediate and the alcohol. However, because more water must be removed in the subsequent process chain to produce the hydrocarbons, the bio-chemical carbon efficiency is lower for this. It follows that biogas is the more inefficient intermediate product although it can be produced more efficiently from biomass. From an energy point of view, the combustion of the solid by-products brings advantages in all considered cases, but in both process routes this heat is also partly sold externally (i.e., heat is available in a surplus).

The results presented are based on the process design and the underlying assumptions of the conversion steps and separation operations. Due to the rather weak data situation, as several process steps have not yet been implemented on an industrial scale, there may be larger uncertainties that have to be taken into account. This applies, for example, to the oligomerization reactions with the focus on kerosene yields. In particular, this uncertainty can lead to the shift of products within the hydrocarbon product spectrum, thus affecting by-product formation. In the various process steps, a trade-off must be made between what is technically feasible and what is economically viable. In the course of this analysis, reference was made to as many processes as possible that have a high degree of technical maturity and thus a certain economic feasibility of these steps seems reasonable. However, since these process

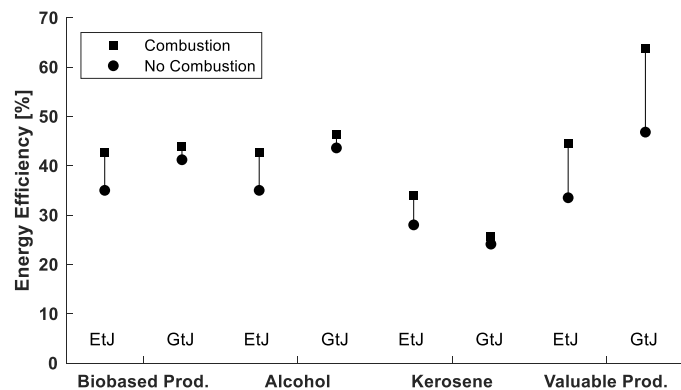


Fig. 11. Energy efficiency with and without solid phase combustion (EtJ: Ethanol to jet; GtJ: Biogas to jet; Prod.: Product).

steps have not yet been assessed, it could, for example, make sense to further reprocess the hydrocarbons to maximize SAF fraction. These include hydrocracking of the higher hydrocarbons and increased direct recycling of the naphtha components.

Based on this analysis, additional interconnection of the plants to increase energy and carbon efficiency should be investigated in further research. In addition, an interconnection of these biogenic processes with a power-based process is promising, as this can increase the carbon yield of the overall process and for the power-based processes the problem of the sustainable carbon source can be reduced. In addition, other feedstocks for SAF production can be analysed with the assessment and modelling approach presented here. Other potentially sustainable feedstocks such as cover crops, solid municipal waste or food waste are available in limited but high quantities. The production of other biogenic intermediates such as butanol or 2,3-butanediol can also be examined to analyse whether higher carbon losses also occur in these intermediates, especially in the biogenic production processes.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgement

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.fuenco.2023.100093](https://doi.org/10.1016/j.fuenco.2023.100093).

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