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Research Report

Production of Greenhouse Gas-reduced or Greenhouse Gas-neutral Gaseous and Liquid Fuels

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Production of Greenhouse Gas-reduced or Greenhouse Gas-neutral Gaseous and Liquid Fuels

Abstract

The use of fuels that are compatible with the existing infrastructure and technology and at the same time have a low or, optimally, no greenhouse gas footprint is an important and arguably indispensable complement to the electrification of the relevant sectors on the path to a greenhouse gas-neutral society.

Within the framework of the project, suitable manufacturing processes and process chains, possible raw materials and products were to be identified and evaluated in terms of potential and social/economic significance using a catalogue of criteria compiled by the DGMK. Possible problems were to be identified and any existing need for research pointed out.

For the different process chains, key parameters such as yield, energy demand, efficiency, land use, greenhouse gas reduction potential or costs were determined, initially on the basis of literature data, later supplemented or replaced by own considerations and calculations. Modular calculation models were developed for this purpose. The aim was to choose the level of detail as fine as necessary and as coarse as possible and thus to enable a comparable procedure and approach for all process chains.

The present study scientifically accompanies and supports the work of the DGMK Research Committee on Greenhouse Gas Reduction.

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Herstellung treibhausgasreduzierter bzw. treibhausgasneutraler gasförmiger und flüssiger Energieträger und Brennstoffe

Kurzfassung

Die Nutzung von Kraft- und Brennstoffen, die mit der existierenden Infrastruktur und Technik kompatibel sind und gleichzeitig einen geringen bzw. im Optimalfall keinen Treibhausgas-Fußabdruck besitzen, stellt eine wichtige und möglicherweise unverzichtbare Ergänzung zu einer Elektrifizierung der entsprechenden Bereiche auf dem Weg zu einer treibhausgas-neutralen Gesellschaft dar.

Im Rahmen des Projektes waren geeignete Herstellungsverfahren und Prozessketten, mögliche Rohstoffe und Produkte zu erfassen sowie hinsichtlich Potenzialen und gesellschaftlicher bzw. wirtschaftlicher Bedeutung anhand eines von der DGMK erarbeiteten Kriterienkataloges zu bewerten. Eventuelle Probleme sollten identifiziert und der ggf. bestehende Forschungsbedarf aufzeigt werden.

Für die verschiedenen Prozessketten wurden maßgebliche Kenngrößen, z. B. Ausbeute, Energiebedarf, Effizienz, Flächenbedarf, Treibhausgasminderungspotenzial oder Kosten ermittelt, zunächst auf der Basis von Literaturangaben, später ergänzt oder ersetzt durch eigene Betrachtungen und Berechnungen. Dazu wurden modular aufgebaute Berechnungs-modelle entwickelt. Ziel war es dabei, den Detaillierungsgrad so fein wie nötig und so grob wie möglich zu wählen und somit eine für alle Prozessketten vergleichbare Vorgehens- und Betrachtungsweise zu ermöglichen.

Mit der vorliegenden Studie werden die Arbeiten des DGMK-Forschungsausschusses Treibhausgasreduzierung wissenschaftlich begleitet und unterstützt.

Berichtsumfang:	113 Seiten, 72 Abbildungen, 38 Tabellen
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Contents

Summary

The use of fuels that are compatible with existing infrastructure and technology, and at the same time have a low or, optimally, no greenhouse gas footprint, is an important and possibly indispensable complement to electrification of the relevant sectors on the way to a greenhouse gas-neutral society.

As a scientific society, the DGMK initiates and coordinates relevant research projects on the production and application of alternative energy sources that can significantly reduce greenhouse gas (GHG) emissions in the fields of action of transport and buildings. To support and scientifically accompany this work, the TU Bergakademie Freiberg was commissioned to prepare a study. Suitable processes and process chains, possible raw materials and products were to be recorded and evaluated in terms of potential and social/economic significance. The study should identify possible problems and show the existing need for research.

For the various process chains, relevant parameters, e.g. yield, energy demand, efficiency, area requirement, GHG reduction potential or costs were determined, initially on the basis of literature data, later supplemented or replaced by own considerations and calculations. Modular calculation models were developed for this purpose. The aim was to select the level of detail as fine as necessary and as coarse as possible, thus enabling a comparable approach and approach for all process chains. The study and the models developed allow holistic system considerations. Model calculations were carried out for various conceivable scenarios and locations, in particular to determine costs, including sensitivity analysis for important influencing variables. The different transport costs were also determined and taken into account.

The studies have shown that even with a very ambitious electrification of transport, significant amounts of advanced fuels will be needed to achieve the climate targets in transport in 2030 without having to accept a major sacrifice in mobility. For the transport demand forecast by the German Federal Ministry of Transport and Digital Infrastructure for 2030 and taking into account 10 million electric vehicles (passenger cars) á 12,000 km/a, greatly improved drive efficiency and modal shift from road to rail, this results in an annual demand of approximately 7.5 million metric tons.

High-quality power and fuel substitutes can be produced on the basis of lignocellulose or carbon dioxide and electricity from renewable sources. Their application properties can be influenced by the process conditions and in some cases exceed the quality of the corresponding conventional products. The manufacturing processes are known in principle and - at least in parts - have already been technically tested on an industrial or demonstration scale. The main obstacles to large-scale application are the lack of viable business models and probably also a lack of political acceptance and support. The manufacturing costs determined for the various process chains and products fit well into the ranges known from the literature. known from the literature. The sensitivity analysis showed that for so-called e-fuels[11] the costs are mainly determined by the electricity or CO2 costs. For biomass-based products, the most important influencing variable is the plant size.

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[1] *e*-fuels: synthetic Fuels based on electrolysis-H_2 and CO_2

Three conceivable production locations with different framework conditions were considered. For Germany, with comparatively high electricity costs, biomass-based energy sources can be produced more economically than e-fuels. Apart from isolated solutions for the production of power-to-liquid products, which can support technology development, the production of electrolysis H2 for hydrogenation processes or fuel cell drives is at best a sensible option from today's perspective. The production of 2nd generation bioethanol from lignocellulose emerged as the most favorable option. Norway offers very good conditions for the production of electricity-based products due to the constant and inexpensive availability of hydropower. A prerequisite, however, is the recovery of carbon dioxide from industrial point sources. In the countries of North Africa or the Middle East, the advantage of low electricity costs is offset by high transportation costs, especially for hydrogen. The separation of carbon dioxide from the atmosphere is very costly. Again, the use of CO2 point sources is an economical alternative.

The studies have also shown that all advanced fuels considered have significant GHG reduction potential compared to the fossil reference (>70 to 95%), even when the GHG intensity of the e-electricity[2] used is included. In cross-comparison, the GHG footprint depends on the yield of target product as well as the GHG intensity of feedstocks. Here, electricity-based products have a slightly higher GHG intensity than biomass-based products. Apart from hydrogen, transport plays only a minor role.

With the final report a generally usable calculation tool (Excel sheet) was handed over, with which the supply costs can be determined for the considered process chains under presetting of variable basic conditions.

Zusammenfassung

Die Nutzung von Kraft- und Brennstoffen, die mit der existierenden Infrastruktur und Technik kompatibel sind und gleichzeitig einen geringen bzw. im Optimalfall keinen Treibhausgas-Fußabdruck besitzen, stellt eine wichtige und möglicherweise unverzichtbare Ergänzung zu einer Elektrifizierung der entsprechenden Bereiche auf dem Weg zu einer treibhausgasneutralen Gesellschaft dar.

Die DGMK als eine wissenschaftliche Gesellschaft initiiert und koordiniert einschlägige Forschungsvorhaben zur Herstellung und Anwendung alternativer Energieträger, mit denen die Emissionen an Treibhausgasen (THG) in den Handlungsfeldern Verkehr und Gebäude signifikant reduziert werden können. Zur Unterstützung und wissenschaftlichen Begleitung dieser Arbeiten wurde die TU Bergakademie Freiberg mit der Anfertigung einer Studie beauftragt. Es waren geeignete Verfahren und Prozessketten, mögliche Rohstoffe und Produkte zu erfassen sowie hinsichtlich Potenzialen und gesellschaftlicher/wirtschaftlicher Bedeutung zu bewerten. Die Studie soll eventuelle Probleme identifizieren und den bestehenden Forschungsbedarf aufzeigen.

Für die verschiedenen Prozessketten wurden maßgebliche Kenngrößen, z. B. Ausbeute, Energiebedarf, Effizienz, Flächenbedarf, THG-Minderungspotenzial oder Kosten ermittelt, zunächst auf der Basis von Literaturangaben, später ergänzt oder ersetzt durch eigene Betrachtungen und Berechnungen. Dazu wurden modular aufgebaute Berechnungsmodelle entwickelt. Ziel war es dabei, den Detaillierungsgrad so fein wie nötig und so grob wie möglich zu wählen und somit eine für alle Prozessketten vergleichbare Vorgehens- und Betrachtungsweise zu ermöglichen. Die Studie bzw. die erarbeiteten Modelle gestatten ganzheitliche Systembetrachtungen. Für verschiedene denkbare Szenarien und Standorte wurden Modellrechnungen insbesondere zur Kostenermittlung einschließlich Sensitivitätsanalyse für wichtige Einflussgrößen durchgeführt. Dabei wurden auch die differierenden Transportaufwendungen ermittelt und berücksichtigt.

Die Untersuchungen haben gezeigt, dass selbst bei einer sehr ambitionierten Elektrifizierung des Verkehrs erhebliche Mengen an fortschrittlichen Kraftstoffen benötigt werden, damit 2030 die Klimaziele im Transport erreicht werden können, ohne dass ein größerer Verzicht an Mobilität in Kauf genommen werden muss. Für die vom Bundesministerium für Verkehr und digitale Infrastruktur für 2030 prognostizierte Verkehrsnachfrage und unter Berücksichtigung von 10 Mio. Elektrofahrzeugen (PKW) á 12.000 km/a, einer stark verbesserten Antriebseffizienz sowie von Verkehrsverlagerung von der Straße auf die Schiene ergibt sich ein Jahresbedarf von ca. 7,5 Mio. Tonnen.

Auf Basis von Lignocellulose bzw. von Kohlendioxid und Strom aus erneuerbaren Quellen sind hochwertige Kraft- und Brennstoffsubstitute herstellbar. Ihre anwendungstechnischen Eigenschaften können durch die Prozessbedingungen beeinflusst werden und übertreffen teilweise die Qualität der entsprechenden konventionellen Produkte. Die Herstellungsverfahren sind prinzipiell bekannt und - zumindest in Teilen - bereits technisch im industriellen oder Demonstrationsmaßstab erprobt. Als Haupthinderungsgründe für eine großtechnische Anwendung stellen sich das Fehlen tragfähiger Geschäftsmodelle und wohl auch eine fehlende politische Akzeptanz und Unterstützung heraus. Die für die verschiedenen Prozessketten und Produkte ermittelten Herstellungskosten ordnen sich gut in die aus der Literatur bekannten Spannbreiten

ein. Die Sensitivitätsanalyse hat gezeigt, dass für sogenannte E-Fuels[21] die Kosten vor allem durch die Strom- bzw. CO_2-Kosten bestimmt werden. Bei biomassebasierten Produkten ist die wichtigste Einflussgröße die Anlagengröße.

Es wurden drei denkbare Produktionsstandorte mit unterschiedlichen Rahmenbedingungen betrachtet. Für Deutschland, mit vergleichsweise hohen Stromkosten, sind biomassebasierte Energieträger wirtschaftlicher herstellbar als E-Fuels. Neben Insellösungen zur Herstellung von Power-to-Liquid-Produkten, die eine Technologieentwicklung unterstützen können, ist allenfalls die Erzeugung von Elektrolyse-H_2 für Hydrierprozesse oder Brennstoffzellenantriebeaus heutiger Sicht eine sinnvolle Option. Als günstigste Möglichkeit zeigte sich die Herstellungvon Bioethanol der 2. Generation aus Lignocellulose. Norwegen bietet aufgrund der stetig undpreisgünstig zur Verfügung stehenden Wasserkraft sehr gute Verhältnisse für die Herstellung strombasierter Produkte. Voraussetzung ist allerdings die Rückgewinnung von Kohlendioxid aus industriellen Punktquellen. In den Ländern Nordafrikas bzw. in Nahost wird der Vorteil niedriger Stromkosten durch hohe Transportkosten insbesondere für Wasserstoff kompensiert. Die Abtrennung von Kohlendioxid aus der Atmosphäre ist sehr aufwendig. Auch hier stellt die Nutzung von CO_2-Punktquellen eine wirtschaftliche Alternative dar.

Die Untersuchungen haben auch gezeigt, dass alle betrachteten fortschrittlichen Kraftstoffe im Vergleich zur fossilen Referenz ein erhebliches THG-Reduzierungspotenzial aufweisen (>70 bis 95 %), selbst wenn die THG-Intensität des eingesetzten *e*-Stroms[32] mit einbezogen wird. Im Quervergleich hängt der THG-Fußabdruck von der Ausbeute an Zielprodukt sowie von derTHG-Intensität der Rohstoffe ab. Dabei besitzen strombasierte Produkte eine etwas höhere THG-Intensivität als biomassebasierte Produkte. Mit Ausnahme von Wasserstoff spielt der Transport nur eine geringe Rolle.

Mit dem Abschlussbericht wurde ein allgemein nutzbares Berechnungs-Tool (Excel-Sheet) übergeben, mit dem für die betrachteten Prozessketten die Bereitstellungskosten unter Vorgabe variierbarer Rahmenbedingungen ermittelt werden können.

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[2] E-fuels: Synthetic fuels based on electrolysis H2 and CO2

[3] *e*-Strom: Strom aus erneuerbaren Energien

1. Introduction

1.1. Task and Procedure

With the climate protection agreement of Paris in 2015, the world community of states committed itself by a large majority to limiting the global temperature increase caused by mankind to below 2, if possible to 1.5 degrees Celsius [1]. This requires a drastic reduction of emissions of so-called greenhouse gases (GHG) such as carbon dioxide, methane or nitrous oxide (laughing gas). The goal is to achieve greenhouse gas neutrality as far as possible in the second half of this century [1], [2].

Against this background, the DGMK has established a Greenhouse Gas Reduction Research Committee. Important goals are to follow and help shape the corresponding political, economic and scientific-technical developments. The DGMK as a scientific society initiates and coordinates numerous research projects to reduce the so-called "GHG footprint" of fuels. This results in the necessity to evaluate new but also already ongoing projects regarding different criteria. To support and scientifically accompany the work of the research committee, the TU Bergakademie Freiberg was commissioned by the DGMK to prepare a study. Suitable processes and process chains, possible raw materials and products are to be recorded and evaluated with regard to potential and social/economic significance. The study is to identify any problems and point out any research needs that may exist.

The basis for the work was the short study "Production of GHG-reduced liquid fuels" (commissioned by the Institute for Heat and Oil Technology IWO e.V.) [3], which was prepared by the TU Bergakademie Freiberg in the first half of 2017 and was to be updated and expanded. Questions of the criteria catalog that had not been considered so far (e.g. opportunities and risks, competing uses, acceptance, integrability into existing processes or plants) were to be included in the considerations, as well as further process chains for the production of gaseous products (hydrogen or methane).

For the various process chains, relevant parameters, e.g. yield, energy demand, efficiency, space requirement, greenhouse gas reduction potential or costs were determined, initially on the basis of literature data, later supplemented or replaced by own considerations and calculations. Modular calculation models were developed. The aim was to select the level of detail as fine as necessary and as coarse as possible, thus enabling a comparable procedure and approach for all process chains.

In the final version, the study and the models developed allow holistic system considerations. Model calculations were carried out for various conceivable scenarios and locations, in particular to determine costs, including sensitivity analyses for important influencing variables.

1.2. Environmental policy objectives and policy framework

As a national contribution to limiting global warming, the German government's Climate Protection Plan 2050 envisages extensive greenhouse gas neutrality in all sectors of society for the second half of this century [2]. At the same time, sector-specific milestones for the reduction of greenhouse gas (GHG) emissions were defined for 2030 in order to achieve this goal (Table 1).

Table 1 GHG reduction targets for 2030 compared to 1990 baseline (D) [2]

Area	**Reduction compared to 1990**
Energy	62 to 61 %
Buildings	67 to 66 %
Transportation	42 to 40 %
Industry	51 to 49 %
Agriculture	34 to 31 %
Total	56 to 55 %

The Climate Protection Program 2030 summarizes a series of measures for implementing the Climate Protection Plan and achieving the targets [4]. One important component is the introduction of CO2 pricing in the sectors not yet covered by the European emissions trading system (non-ETS sector). In addition to parts of industry and agriculture, these include above all the areas of transport and buildings. Furthermore, fields of action are defined with which a significant reduction of GHG emissions can be achieved. In the transport sector, these include:

- Shift to climate-friendly alternatives (rail, inland waterways, cycling),
- Use of alternative fuels (electricity-based fuels, advanced biofuels),
- shift to other propulsion systems, and
- digital networking.

The buildings sector includes building heating and cooling as well as water heating (households, commerce, trade, services, public buildings). Important measures to reduce emissions include increasing energy efficiency (e.g., energy-efficient building refurbishment, replacement of heating systems) and expanding the use of renewable energies.
The most important measures to reduce emissions include increasing energy efficiency (e.g., energy-efficient building renovation, replacement of heating systems) and expanding the use of renewable energies.

The Federal Climate Protection Act, which came into force on December 18, 2019, is intended to ensure that national climate targets are met. Permissible annual emission levels have been set for the period 2020 to initially 2030 in the areas listed in Table 1 (see Annex 1). Responsibility for compliance lies with the relevant federal ministries. If necessary, they must ensure that the emission limits are not exceeded by means of suitable emergency programs.

In addition, there are several directives, laws and regulations that are intended to help meet European and national climate protection targets. These include the EU's Renewable Energies Directive (and its transposition into national law in the BImSchG and the 37th BImSchV). There are minimum shares of renewable energy in final energy consumption, quotas for alternative fuels and energy sources, but also specific GHG reduction targets. The most important environmental policy and legal framework conditions for reducing energy consumption and

GHG emissions in the transportation sector are summarized in Table 2.

Table 2 Environmental policy and legal framework[4]

Parameter	2020	2030	Quelle
Reduction of GHG emissions (reference year 1990) - total - in transport	40 %	55 % → 65 % 40 % → 48 %	Climate Protection Plan Draft: Amendment to Climate Protection Act 5/2021
GHG reduction road transport (reference value 94,1 kg CO_2-eq/GJ)	> 6 %	> 25 %	BImSchG 2015 Draft: Act on the further development of the GHG reduction quota 2021
Share of renewable energy in final energy consumption (total)	> 20 %	> 32 %	Renewable Energies Directive RED I 2009/2015 resp. RED II 2018 38th BImSchV 2021
Share of renewable energy in final energy consumption in transport (road + rail)	> 10 %	> 14 %	
thereof - Conventional biomass (food and feed crops)	max. 7 % (EU) < 6,5 % (D) 1)	< 4,4 % (D) 1)	
- advanced biomass (credit factor 2 2))	> 0,5 %	> 2,6 %	
- Fuels from used cooking oils and animal fats		< 1,9 %	
Biodiesel in DK Paraffinic fuels in DK	< 7 % (v/v) < ≈26 % (v/v)		Fuel quality guideline (FQD 2015) Fuel standardization (DIN EN 590 and 228)
Oxygen content in OK	< 2,7 % (m/m) < 3,7 % (m/m) (E10)		
Fleet limit value (CO2 emissions)	95 g/km (NEFZ-Basis)	37,5 % less than 2020 (WLTP-Basis)	EU Decision 443/2009 EU Decision 12/2018

1) national determination 2) for the share exceeding the minimum share.

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[4] Changes in GHG reduction rate from 22 to 25% and increase in GHG reduction targets under Climate Change Act to 65% (total) and 48% (transportation) only after copy deadline.

The overarching goal of the energy turnaround is to reduce GHG emissions. With reference to 1990 reference values, the values of 55% (total) and 40-42% (transport sector target) stated in the Climate Protection Plan for the year 2030 are absolute values[5]. In contrast, the minimum shares of renewable energy in final energy consumption (gross) stipulated in the EU Renewable Energy Directive are relative requirements. The same applies on the vehicle side for the so-called fleet limit values (weighted average values of the standard emissions of new vehicles according to registration numbers). These values are used for control purposes; however, compliance with them does not guarantee that the GHG reduction targets will be met.

Advanced fuels also include electricity-based synthetic fuels. However, according to the regulations of the 37th BImSchV, these are only recognized as renewable if they are either produced in plants that are disconnected from the power grid or are operated exclusively with otherwise regulated surplus electricity from renewable energy plants.

An amendment to the Renewable Energy Directive in 2015 brought into focus possible indirect land use changes that could theoretically lead to high GHG emissions despite the use of sustainably grown biofuels. Individual member states have since been able to set caps on conventional agriculturally produced biofuels. In addition, biofuels that do not compete with food production in terms of land use, such as fuels from residues or algae, as well as electrically powered vehicles, are to receive special support.

Further specifications relate to the minimum proportion of so-called advanced biofuels from non-food biomasses as well as the upper limits for biofuels from food and fodder crops or waste oils (used cooking oils and animal fats). Furthermore, in addition to various crediting factors, the Fuel Quality Directive and the standards for fuels must of course also be taken into account.

1.3. Situation in the Transport Sector

1.3.1. GHG emissions in transport

Figure 1 shows the development of GHG emissions for selected sectors since 1990 in Germany. The transport sector accounts for about one fifth of energy-related emissions in Germany. However, while significant reductions have already been achieved in the energy sector (-30%) and buildings (-40%), transport related GHG emissions remain almost unchanged at 163 million metric tons of CO2 equivalent (Figure 1). Therefore, transport in particular, is in the focus of political and public discussions.

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[5] When calculating sector-specific emissions, only the GHGs generated directly by the combustion of fossil fuels are considered. The other GHG emissions generated during fossil fuel extraction and processing, electricity generation for electric vehicles, and biomass cultivation and processing into biofuels are allocated to other sectors.

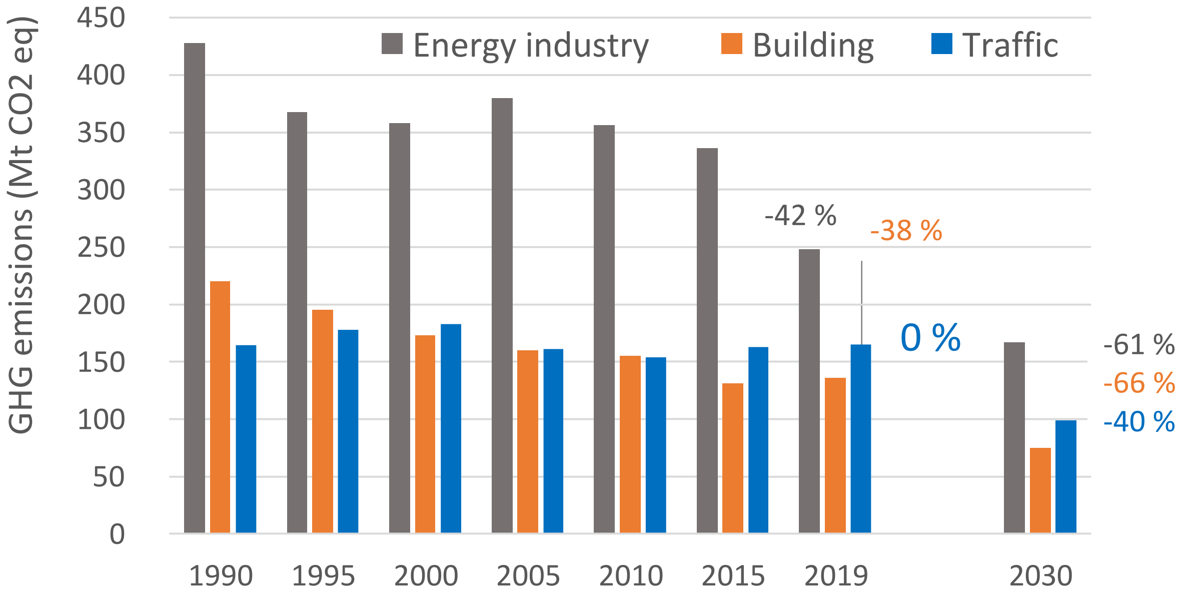

Figure 1 Development of greenhouse gas emissions in Germany [2], [5]

In addition to the GHG intensity of the energy sources used, the absolute transport-related GHG emissions also depend decisively on the energy demand in the transport sector. This is determined by the necessary transport services and the energy efficiency of transport. In Germany, the trends were in the opposite direction. The specific fuel consumption of the passenger car fleet has fallen by almost 20% since 1990, from 9.1 l/100 km to 7.4 l/100 km [6]. However, this is compensated by a strong increase in transport volume (passenger- or tonne-kilometers) (passenger transport: +37 %, freight transport: +75 %) [6], so that final energy demand and thus GHG emissions in the transport sector have hardly changed since 1990.

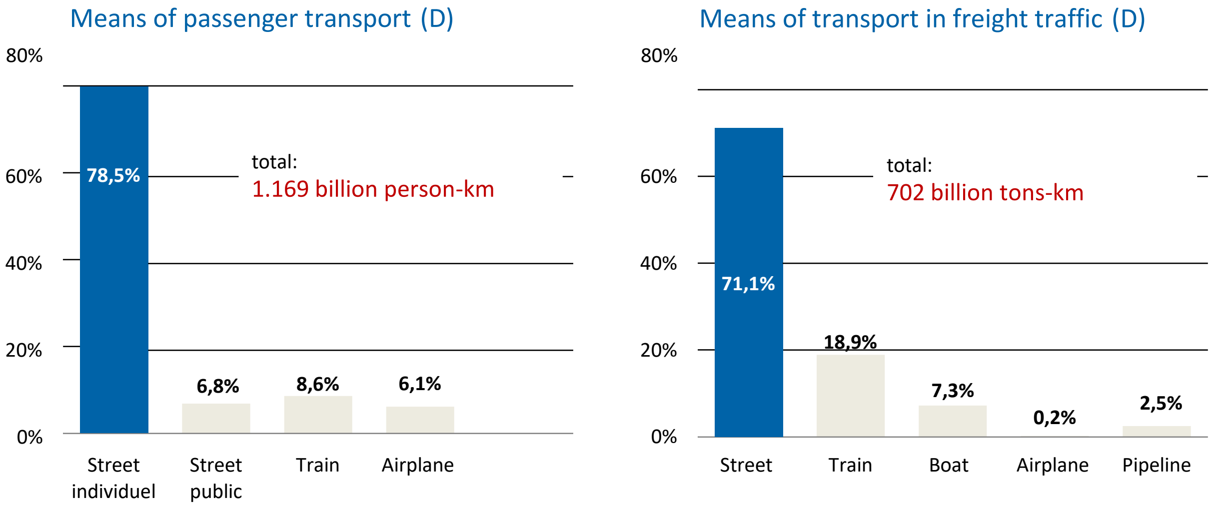

Figure 2 Transport needs and means of transport in Germany (2017) [6]

As Figure 2 illustrates, the vast majority of traffic in Germany is currently carried by road, with private transport in particular accounting for a significant share of transport performance and the associated CO2 emissions. The share of freight transport in transport-related final energy consumption is about 30 % [6].

1.3.2. Traffic development

The demand for transport has grown steadily and strongly since 1990, in passenger transport by almost 35 % and in freight transport by as much as approx. 75 %. According to most available forecasts, this trend will continue in Germany and the other EU member states in the future. Regardless of the corona-induced decrease in transport volume in 2020, relatively strong increases are forecast for freight transport in particular [6], [7].

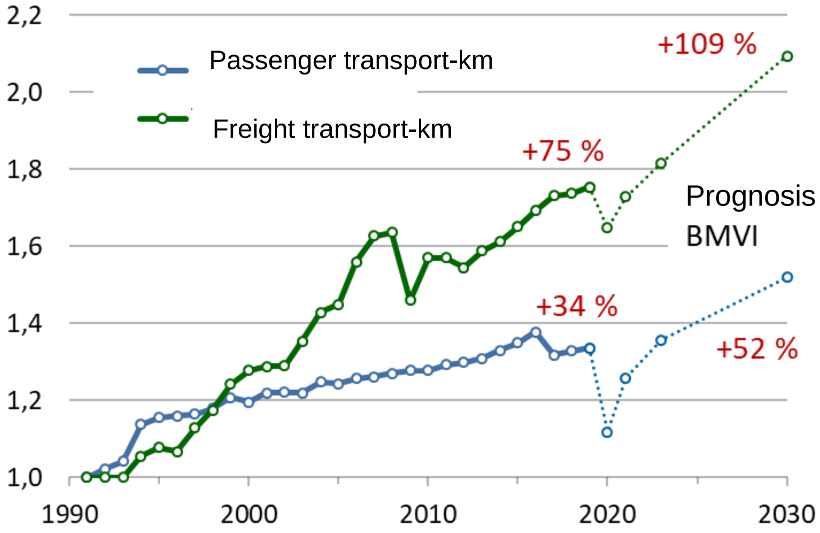

Figure 3 Development of traffic (relative) in Germany and forecast according to [6]

In a study commissioned by the Research Association for Combustion Engines (FVV) entitled "Renewables in Transport 2050" [8], a distinction is made between

- a scenario with high mobility demand, in which both passenger and freight transport show high growth rates, and
- a low mobility demand scenario, in which an increase in freight traffic in Germany is offset by a decrease in passenger traffic Table 3.

Table 3 Changes in mobility demand in Germany up to 2050 (Basis 2010)

Changes 2010 to 2050		**Germany**	**EU**
High mobility demand	Passenger traffic	+ 30 %	+ 50 %
	Freight traffic	+ 60 %	+ 80 %
Low mobility requirements	Passenger traffic	- 25 %	+ 10 %
	Freight traffic	+ 20 %	+ 50 %

The German Federal Ministry of Transport and Infrastructure (BMVI) forecasts an increase for 10% in passenger transport and 17% in freight transport by road by 2030, based on 2010 [6]. In air transport (domestic and international), an increase of 65% in passenger traffic and 92% in air freight traffic is expected by 2030 compared to 2010 [9].

From today's point of view, possible drive systems for road vehicles are internal combustion engines and electric motors, each of which can act as the sole drive unit or - in the case of hybrids - together. - or, in the case of hybrids, together. Liquid or gaseous (H2, methane, liquid gas) fuels or electrical energy can be used as energy sources. Currently, the use of internal combustion engines and liquid fuels is dominated.

The structure of the vehicle population for the year 2050 and thus also the future demand for the different energy sources is determined by many technical and political framework conditions and can hardly be reliably predicted at present. The BDI study "Climate Paths for Germany" assumes for its climate protection scenarios that only battery-electric vehicles will be registered in 2050.

In contrast, other studies consider several scenarios for the development of the vehicle population. For example, the study commissioned by the FVV [8] considers a balanced (FVV), an electrified (EMob), and a combustion scenario (PtL) (see Figure 4). Analogous scenarios can also be found in the dena lead study [10].

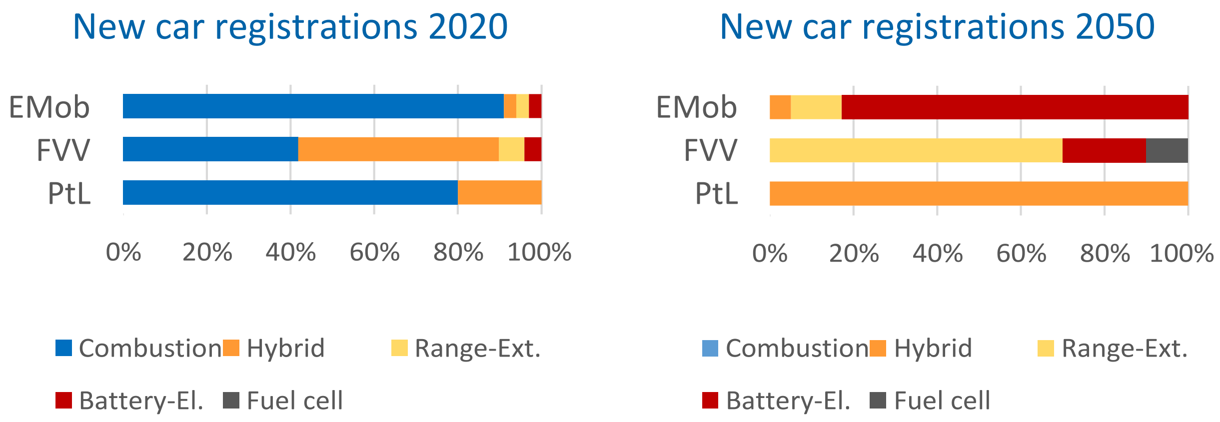

Figure 4: New registrations by mode driving 2020 and 2050 [8]

These forecasts also agree that no new vehicles equipped exclusively with internal combustion engines will be registered in 2050. However, hybrid solutions play a strong role in the concepts studied. Even the electromobility scenario of the FVV study considers a market share of just under 20% for hybrid or range extender solutions.

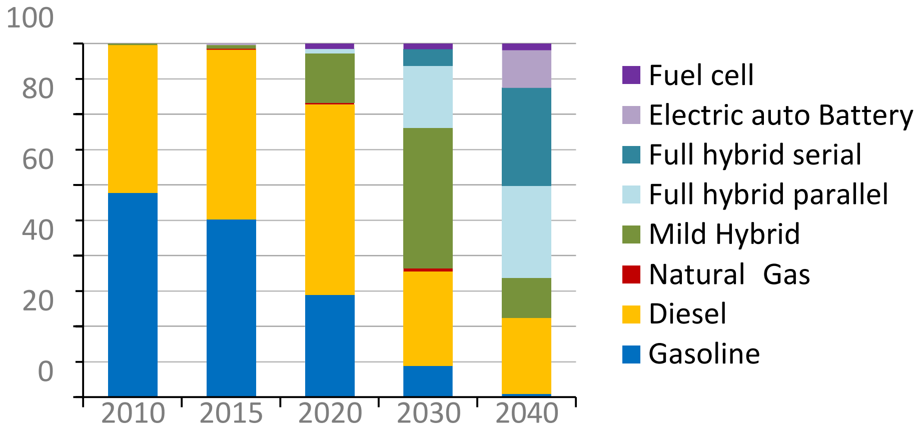

Figure 5 Development of new passenger car registrations by drive type (D) [11]

Similar results were reached by DLR in its 2013 study [11], in which hybrid vehicles are also predicted to dominate future motorization in the passenger car sector (Figure 5). Hydrocarbon-based fuels will still be needed in 2050 to supply both new cars equipped with combustion engines and existing vehicles with energy. In addition, there will be a need for areas for which no alternative solutions are conceivable from today's perspective (air transport, maritime transport). However, in order to achieve GHG reduction targets in the future, carbon cycles must be closed, thus avoiding GHG emissions associated with the production and use of fuels.

1.4. Demand for advanced fuels and combustibles

The prerequisite for political decisions and investment planning is knowledge of future fuel and energy requirements for achieving energy policy goals. This results from the expected traffic volume as well as from the type of means of transport used or the degree of electrification in road transport. Outside the transport sector, "GHG-reduced" fuels can be used in the heating sector as a substitute for heating oil or natural gas. Another important application specifically for PtX products[6] is the chemical storage of electrical energy and reconversion to electricity during a so-called "dark period".

1.4.1. Future fuel demand - results of various studies

A number of studies have dealt with the forecasting of fuel and energy demand and predicted corresponding developments for different scenarios [12], [10]. There is a consensus that liquid and gaseous hydrocarbons will continue to be indispensable in the future, but the quantities of GHG-reduced energy sources required differ greatly in some cases (see Figure 6).

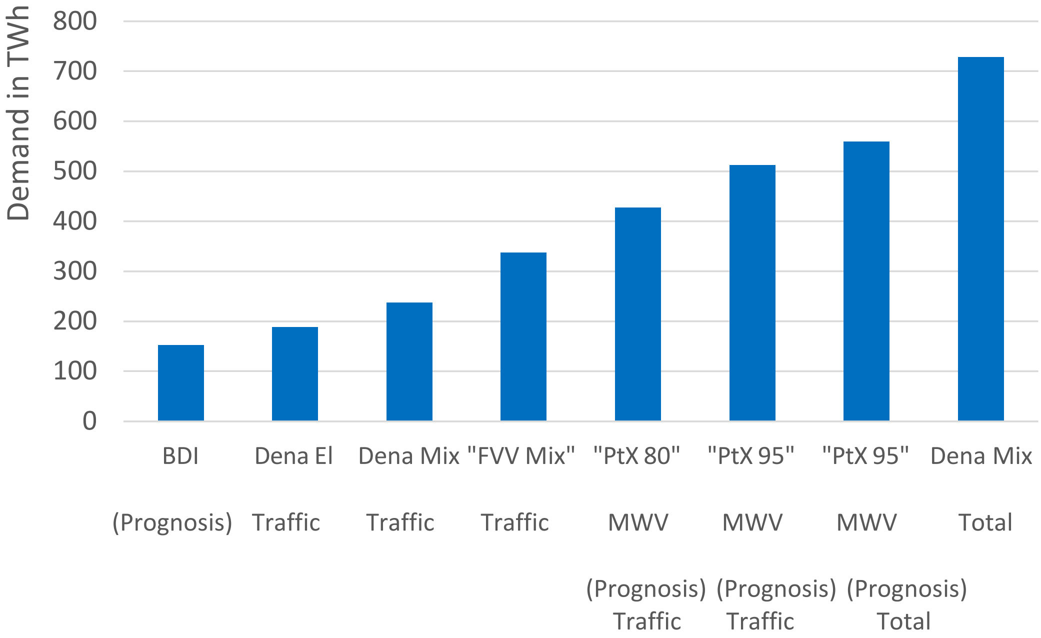

Figure 6 Demand for advanced fuels in 2050 (D)

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[6] PtX: Power to "X" - electricity-based synthetic gaseous or liquid energy carriers

The relatively wide range results from the different basic assumptions and approaches of the studies. For example, the study commissioned by MWV [12] is a study with an exploratory scenario, in which it is investigated how the climate protection targets can realistically be achieved with the help of PtX technologies. However, it does not examine whether there may be more favorable options for achieving the targets. The study initiated by the BDI [13], on the other hand, examines normatively how the climate protection targets can be met most efficiently with the defined basic assumptions. Since a direct use of electricity in the transport sector is associated with a higher efficiency than the use via PtX, the amount of battery electric vehicles and trolley trucks is widely used in this study. It does not consider whether implementation is realistic or feasible. In the studies of FVV [8] and dena [10], various exploratory scenarios are considered equally alongside each other, including scenarios with extensive use of PtX fuels, but also scenarios with extensive electrification, in which the use of synthetic fuels is correspondingly lower.

In these studies, the areas of application for PtX products in transport relate predominantly to air and marine transport, where it is not foreseeable that there will be an alternative to the use of liquid fuels in the future. Liquid fuels will also continue to dominate in heavy-duty vehicles, even though trolley trucks play a not insignificant role in individual studies. Only in the case of light commercial vehicles and especially passenger cars is a switch to battery electric vehicles seen to varying degrees by 2050. Nevertheless, even then the stock will still include many vehicles with combustion engines.

1.4.2. Modeling of energy and fuel demand

However, given the very different targets and limitations, the exact fuel requirements are not obvious from the various studies. In particular, the question of how different technical and energy policy measures affect the demand for advanced fuels is not answered. Therefore, a 2-step calculation tool was developed in this thesis to determine the future energy source and fuel mix for a wide variety of framework conditions.

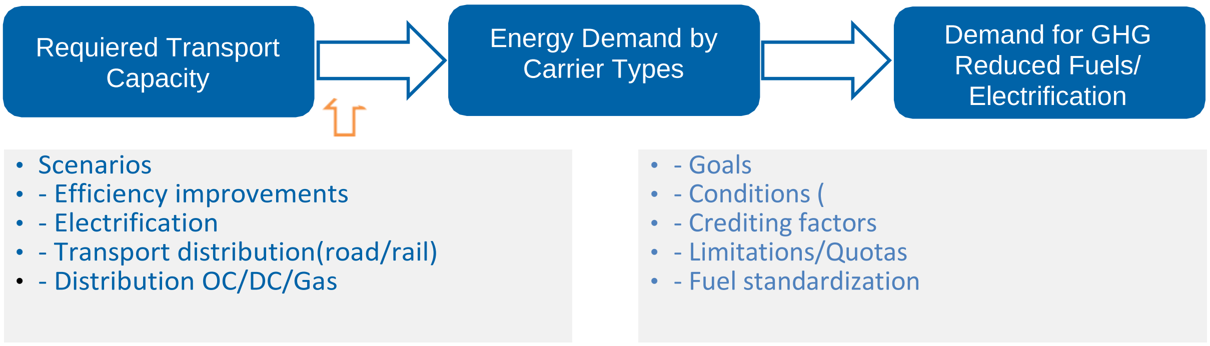

Figure 7 Scheme of modeling fuel demand

Figure 7 schematically shows the procedure for modeling the demand (see also Appendix 2). First, based on a required transport capacity, the energy demand is determined, broken down by energy carrier types (DK, OK, gases, electricity). For the consideration of different scenarios, the degree of electrification, the distribution among different means of transport and, if necessary, efficiency improvements can be specified or varied. In the second step, a fuel/energy carrier mix is then quantified in detail, which also includes the required quantities of GHG-reduced fuels and/or the degree of electrification for meeting the climate targets.

GHG emissions from transport are largely determined in absolute terms by energy consumption and thus by the transport performance achieved. In order to illustrate the influence of transport demand on the amount of advanced fuels required to meet climate targets and to show the effects of various measures, the calculation parameter "wheel energy" was introduced. This is the amount of energy that must be available at the drive wheels to propel the vehicle. With the help of the wheel energy, different transport performances (passenger or ton kilometers) in road and rail transport can be linked to an energy requirement. This quantity is independent of efficiency, so that drive systems with different efficiencies can be considered. The methodology for determining the wheel energy is described in Annex 4.

In the following figures 8 to 10, the demand for advanced fuels for different scenarios is plotted as a function of transport performance (relative: 2017 100%). These quantities should be considered as additional requirements to all other fuels and energy carriers (fossil fuels, conventional biofuels, electricity for rail and road), which are not shown in the figures. They are required to meet climate targets7 for a given transport performance. The vertical red lines embody the current (100%) and projected 2030 transportation demand. The intersection with the advanced fuel demand trajectories characterizes the respective operating point. Figure 8 (left) shows the advanced fuel demand to meet the 22% target (green line) and the 40% target (red line) as a function of transportation capacity. With today's mobility demand, reducing GHG intensity in transport by 22% is not sufficient to meet the 40% target of the Climate Change Act (point 1). As an absolute target, the 40% reduction in GHG emissions from the 1990 baseline could be achieved simply by foregoing approximately 40% transportation service. However, this would miss the 22% target (point 2). For a 22% reduction in GHG intensity of fuels to be sufficient to meet the 40% target, transportation services would need to be reduced by about 35%, while at the same time the use of advanced fuels is required (point 3). The courses of the green and red lines now result in the blue demand curve for meeting the climate targets shown in the figure on the right. Here, we first assume today's transportation demand and project the current level of development into the future. The expected increase in transportation demand moves the operating point on the blue line to the right; advanced fuel demand would increase from about 930 PJ to 1,215 PJ (about 27 million tons). The total transportation-related final energy demand is 2,750 PJ.

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[7] Amendment to the federal Climate Protection Act not until after the editorial deadline (the bills presented relate to the goal of reducing GHG emissions in transport by 40% compared to 1990); increase in the GHG reduction quota under the Act to further develop the GHG reduction quota from 22% to 25% also after the editorial deadline.

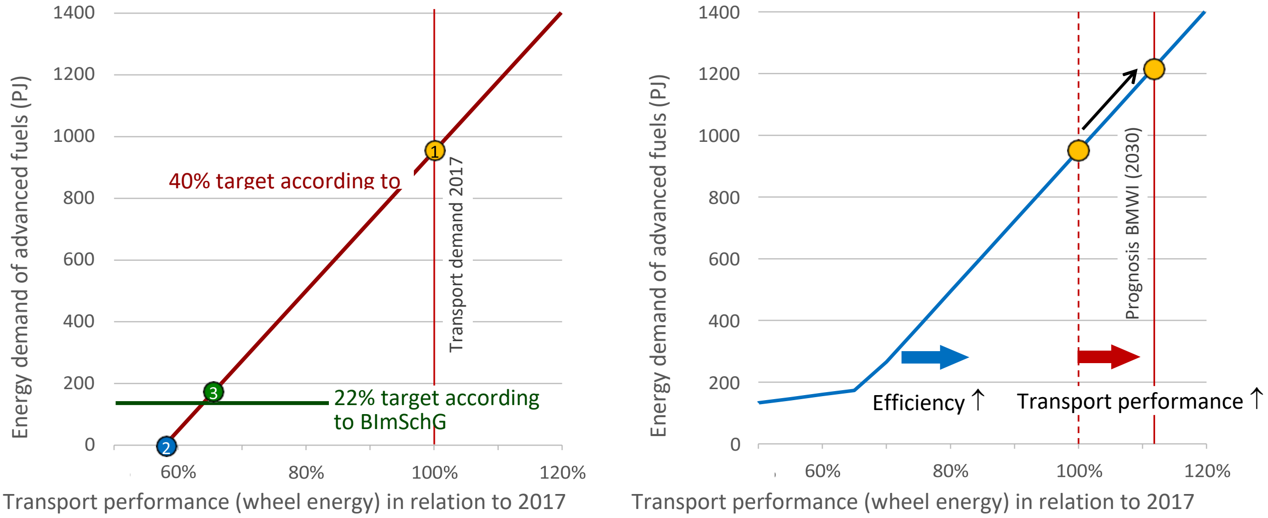


Figure 8 Need for advanced fuels to achieve the 40% target for 2030 (excluding e-mobility)

Improvements in the efficiency of internal combustion engines would be visible in this diagram by a shift of the blue curve to the right and a somewhat smaller increase. At present, specific fuel consumption for new passenger cars is 4.9 l/100 km (diesel) and 5.6 l/100 km (gasoline), around 25 % below the current fleet average (7.4 l/100 km). Due to the increasing replacement of old vehicles, the fleet average consumption will continue to decrease in the coming years, so that significant improvements in the efficiency of the drive technology of internal combustion engines can be assumed by 2030. The illustration in Figure 9 (left) is based on efficiency increases of 20% for passenger cars and 10% for trucks. This is associated with a decrease in the required amount of advanced fuels by ≈ 35 % to 800 PJ (total transport 2,150 PJ).

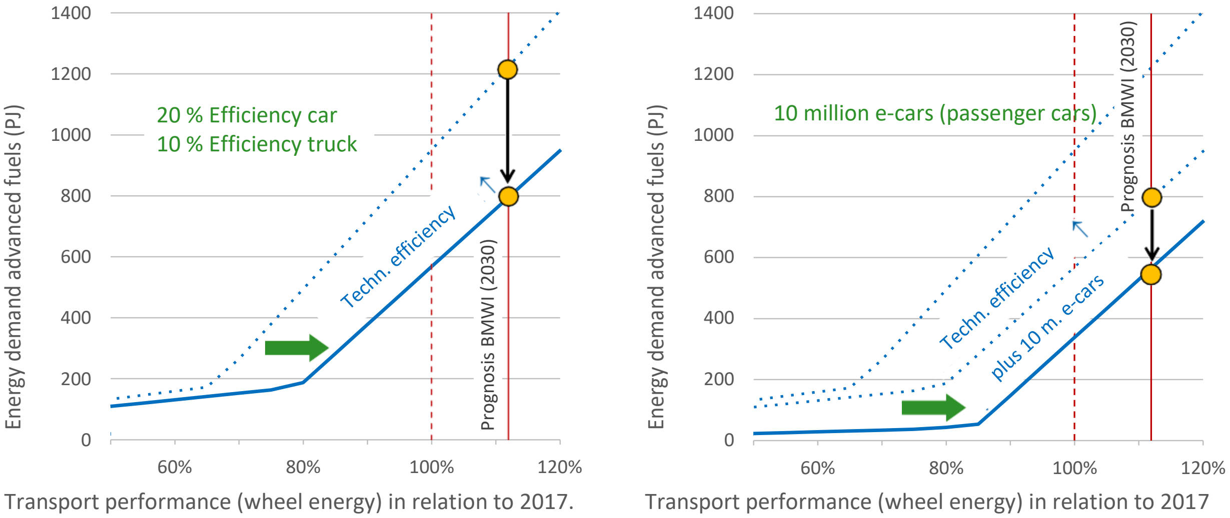


Figure 9 Need for advanced fuels to reach the 40% target for 2030 (with efficiency improvements, and e-mobility).

The next step is to show how increasing market penetration with electric vehicles will affect the additional demand for advanced fuels to meet the climate targets (40% target). For the calculations, a very ambitious electrification with 10 million e-cars (12,000 km/a, 25 kWh/100 km) in 2030 was assumed. As Figure 9 (right) shows, the demand for advanced fuels could thus be reduced by 255 PJ to 545 PJ while transport capacity remains unchanged. However, this is also associated with an additional electricity demand of about 110 PJ. The higher efficiency of electric drives (tank-to-wheel) further reduces the total energy demand to 1,980 PJ.

Other opportunities that can be used to achieve a reduction in GHG emissions include improvements in logistical efficiency. This includes, for example, measures to shift traffic from road to rail or from private to public transport, or better vehicle utilization. The effect of all this is that a certain transport service can be provided with a lower energy input (wheel energy).

For the scenario shown in Figure 10 (left), it was assumed that 10% of individual passenger transport and 10% of freight transport could be shifted to rail. This would mean roughly a doubling of the current passenger transport performance of the railroads in local and long-distance traffic. In the chart, the red demand line now moves to the left. Advanced fuel demand decreases by 212 PJ to 333 PJ. This is equivalent to about 7.5 million tons of fuel. The new operating point (green) is slightly below the blue demand curve. This is due to the fact that the shift to rail causes the (not shown) demand for traction power to increase (46 -> 86 PJ) and at the same time the demand for fuels to decrease.

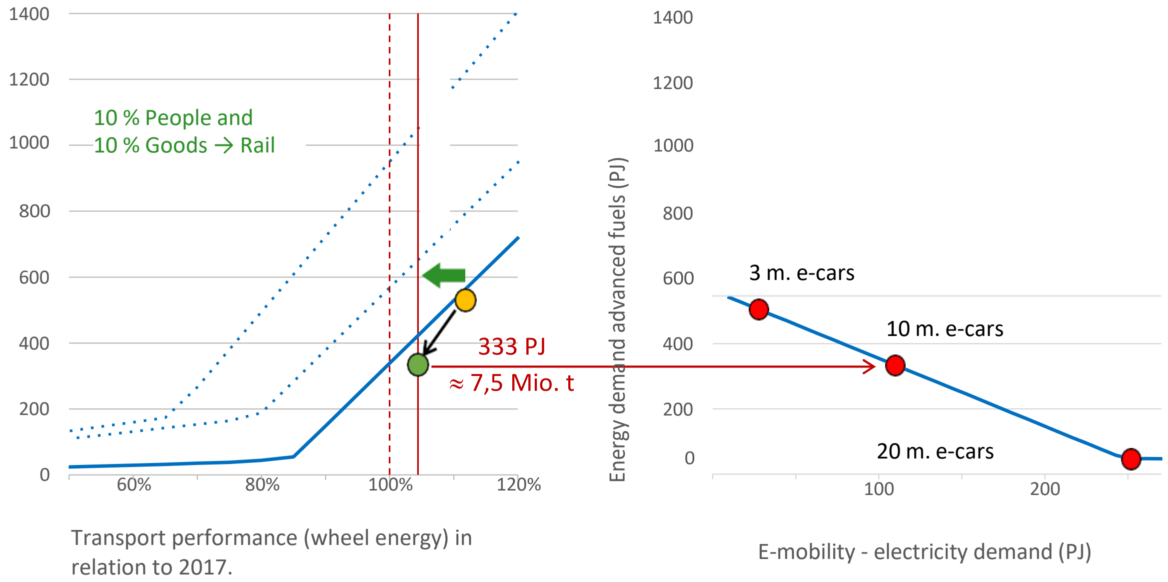


Figure 10 Demand for advanced fuels to reach the 40% target for 2030, left: Impact of shift to rail (with efficiency improvements, with e-mobility), right: with variable electrification in the same scenario.

Projecting this demand into the right-hand graph of Figure 10 illustrates the impact of electric vehicle market penetration on liquid advanced fuel demand. If fewer than 10 million electric cars are put on the road, the demand for liquid "GHG-reduced" fuels continues to increase. To get by for the outlined scenario without out-of-plan advanced fuels, about 20 million electric cars with an average annual mileage of 15,000 km would be needed. To meet the 48%

reduction in GHG emissions from transportation compared to 1990 called for in the Climate Protection Act amendment, the demand for advanced fuels was projected to increase from 333 PJ (7.5 million metric tons) to 510 PJ (about 12 million metric tons).

With the partly very drastic measures shown (20% increase in efficiency of combustion engines, 10 million e-cars, shifting 10% each of freight and passenger transport performance to rail), total final energy consumption in road and rail transport can be reduced by 20% to about 1,980 PJ compared to 2017 (2,486 PJ [14], [15], [16]). In these calculations, the predicted increase in transport performance has already been considered. Due to the assumed strong electrification of transport as well as the assumed modal shift, the electricity demand in the transport sector increases to almost 200 PJ (road: 110 PJ, rail: 86 PJ). This leaves a demand for liquid fuels of about 1,785 PJ. To achieve the required reduction in GHG emissions, significant amounts of alternative advanced fuels with a low carbon footprint are needed to substitute fossil shares, as illustrated in Figure 10. Figure 11 shows an example of a possible composition of such fuels.

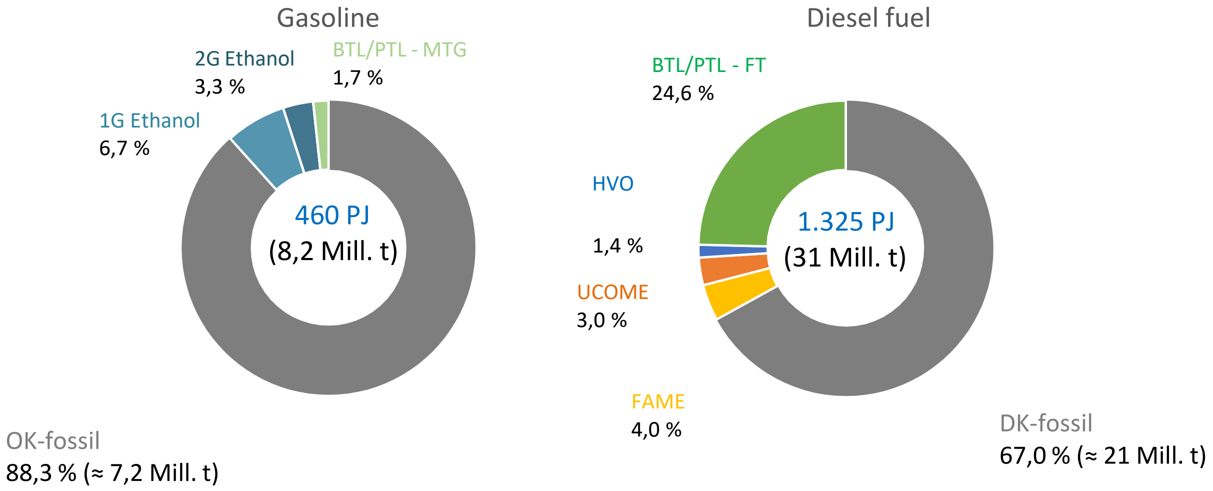


Figure 11 Exemplary fuel composition (D, 2030) for meeting the 40% target (vol.-%)

The calculations carried out may be somewhat striking and are intended, in particular, to show the effects of various measures to reduce GHG emissions. They do not fulfill the claim to consider or even predict all subtleties of future developments. However, they do illustrate the dimension of the task facing the transport sector in connection with meeting climate targets. Electromobility will occupy an important position in a future transportation system. However, achieving the 2030 GHG emissions reduction target will also require the use of existing infrastructure in conjunction with the introduction of advanced liquid fuels. The alternative to this would be drastic changes in society, in particular a noticeable restriction of individual road traffic.

1.4.3. Market launch

The production capacities required for the manufacture of advanced fuels cannot be made available "right away". Rather, starting from initial demonstration and production facilities, there is an increasing market penetration. Historical ramp-up curves often show an exponential progression. For example, for ammonia production using the Haber-Bosch process, capacity has doubled approximately every 5 years [17]), and for coal hydrogenation using the Bergius-Pier process, every 4 years [18]. For the estimation of the technology ramp-up for advanced fuels, a capacity doubling every 2 years was assumed and thus a similar development as for photovoltaics [19].

In the calculations, a hypothetical 2030 demand of 333 PJ was initially assumed, based on the assumptions presented above (Figure 12, orange curve). For this capacity to be available in 2030, plants with a production of around 10 PJ would have to be in operation today if capacity were doubled every 2 years.

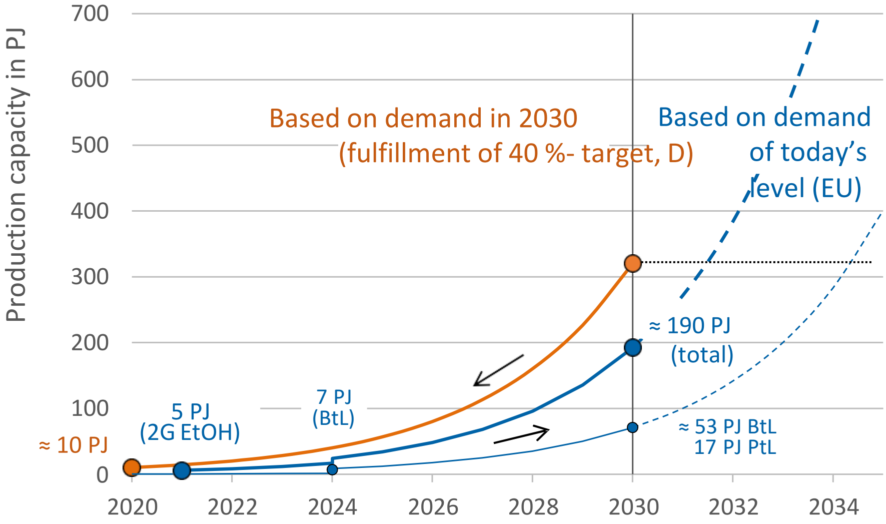


Figure 12 Market launch -forecast ramp-up curves

Except for a small PtL plant in Iceland for the production of methanol [20], only a few - mostly sporadically operated - demonstration plants currently exist, so that there is an urgent need for action, even taking into account the necessary planning and approval phases. To estimate the development of production capacities, at least roughly, for advanced fuels, assumptions had to be made regarding the commissioning of the first production plants. For example, Sunfire plans to produce e-fuels in a small plant (8 kt/a) in Norway from 2020 onwards, based on Fischer- Tropsch synthesis [21]. In the field of BtL technologies, the French BioTFuel project [22] is in the planning phase for a 200 kt/a plant (7 PJ/a). For the calculations, a completion by 2024 was assumed. In contrast, several plants are or were already in operation to produce cellulosic ethanol (2G ethanol) [23]; additional plants in Romania, Finland, and Slovakia are scheduled for commissioning in 2020/2021 with a total capacity of approximately 200 kt/a [24]. The market ramp-up estimate based on this is shown in Figure 12. In the cumulative plot, the thicker blue line shows the total capacity to produce 2G- Ethanol and synthetic fuels (BtL and PtL), respectively. Until 2024, the progression is mainly based on the development for ethanol only; with the commissioning of the BioTFuel plant, the market penetration with synthetic fuels will then also start. Based on these assumptions, production capacities for advanced fuels of just under 200 PJ could be created in Europe by 2030. Of this, synthetic fuels account for about 70 PJ. However, these estimates are extremely influenced by the initial conditions chosen (year and capacity) and are thus subject to large uncertainties. Regardless, the results indicate that there will not be sufficient production capacity for advanced fuels by 2030. However, due to the exponential nature of such ramp-up curves, large capacity increases can be expected within just a few years once the market ramp-up is underway. This is clearly illustrated by the right-hand part of Fig. 12. However, an essential prerequisite for this is that there is also a driving force for this development. In addition to the need to reduce greenhouse gas emissions, there must also be an economic business model for potential investors or operators of such plants.

Hydrogenated vegetable oils (HVO) show excellent application properties [25], [26], [27] (see section 4.2.2). In a certain transition period, the coverage gap for advanced fuels could be closed by using HVO. It is true that the creditability of HVO for meeting the 22% target is limited by the provision of RED II. However, higher percentages are possible and can help mitigate GHG emissions. Hydrogenated vegetable oils can be produced relatively inexpensively both in stand-alone plants and through co-processing in petroleum refineries. In recent years, this technology has developed rapidly. By 2020, the production capacity for HVO in Europe was expected to be 3.87 million t/a [28].

1.5. Interim summary

Although the transport sector is responsible for only about 20% of Germany's total current CO2 emissions, the reduction of transport related GHG pollution is an immense challenge due to the large absolute quantities involved. To achieve climate protection targets, all options for reducing the CO2 footprint of transport must be exploited. Even with a very ambitious electrification of transport, the striking estimate for 2030 presented here results in a need for advanced fuels of 7.5 million tons, without which the transport targets (40% reduction of GHG emissions compared to 1990) will not be met. Synthetic products based on biomass or renewable electricity and carbon dioxide, together with 2nd generation bioethenol, have the necessary potential. In addition, conventional or other biofuels can and must also make an important contribution within the scope of their (limited) approval or availability. So far, there are only demonstration plants for the production of synfuels, although the technical know-how is available in principle. There is thus an urgent need for action to ensure that the necessary capacities can be created by 2030. Experience shows that ramp-up curves for the introduction of new technologies into the market have an exponential course. Thus, there is a realistic possibility of catching up with delays within a few years.

2. Raw materials

2.1. Raw material sources - overview

Gaseous and liquid fuels are mostly organic substances or mixtures of substances that are mainly composed of the elements carbon and hydrogen (hydrocarbons). Other elements (heteroelements) such as sulfur, nitrogen or oxygen are generally undesirable and are tolerated only in traces by corresponding standards. An exception are some oxygen-containing components, which can have positive effects on product properties (anti-knock properties of OC, emission reduction) and are permitted in certain proportions (e.g. ethers, alcohols or biodiesel).

Crucial for the climate impact is the origin of the main elements carbon and hydrogen. In addition to fossil energy sources (mineral oil, natural gas, coal), on the basis of which conventional fuels are mainly produced, other raw material sources come into consideration, especially from the point of view of sustainability:

- Carbon: biomass, carbon dioxide from point sources or the atmosphere, biogas, organic waste.
- Hydrogen: biomass, biogas, organic waste, water (electrolysis), (conventionally produced hydrogen coupled with CO2 storage).

The use of alternative fuels also ultimately results in combustion to water and carbon dioxide. In contrast to fossil raw materials, the carbon is incorporated promptly via the path of photosynthesis or through the direct use of carbon dioxide, so that the carbon cycles are closed (GHG neutrality). However, the extraction of alternative raw materials as well as their processing and transport are associated with energy expenditures and emissions that must be considered in a greenhouse gas balance (CO2 footprint).

2.2. Biomasses

Chlorophyll-containing plants are able to synthesize energy-rich organic substances (carbohydrates, fats, proteins) from carbon dioxide absorbed from the atmosphere and water, using the sun's radiation energy. Biomasses can therefore in principle be regarded as renewable sources of carbon or hydrogen.

Potential

The potential for domestic bioenergy is estimated by the Fachagentur Nachwachsende Rohstoffe e.V. (Agency for Renewable Resources e.V.) (FNR) estimates the potential for domestic bioenergy. For the year 2050, the total potential is estimated at about 1,800 PJ (Figure 13 and Appendix 3) [29]. Energy crops (e.g., corn, rapeseed, beets, cereals, grasses) account for the largest share of this, with 732 PJ, which are grown on agricultural land. This estimate is based on a cultivated area of 4 million hectares available for this purpose (currently 2.4 million hectares). Today, only one-third of this potential has been utilized. For straw, which has hardly been used for energy, the potential is 142 PJ and for liquid manure and dung 114 PJ. This results in a total potential for energy from agriculture of just under 1,000 PJ. In addition, residual wood from forestry or landscape conservation contributes about 400 PJ to the bioenergy potential (about 40 % not yet used). Industrial residual wood and waste wood (approx. 220 PJ), on the other hand, as well as residual and waste materials from the food and animal feed industries, are already being used almost completely for energy production.

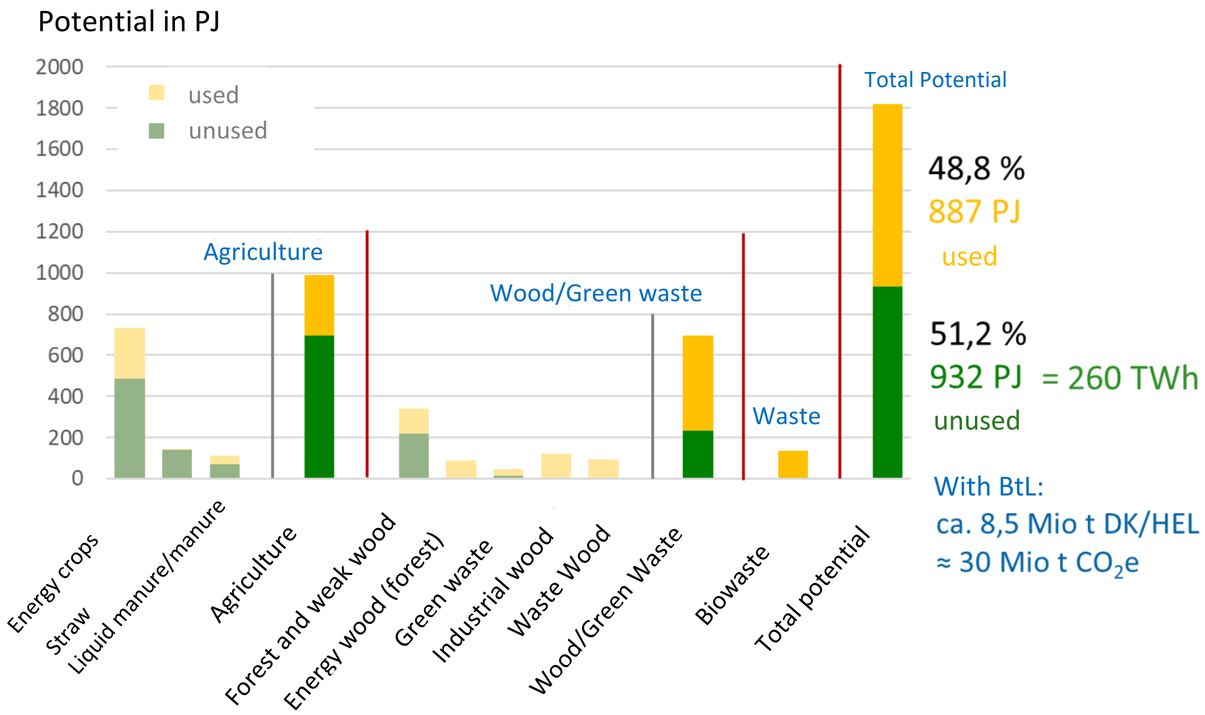
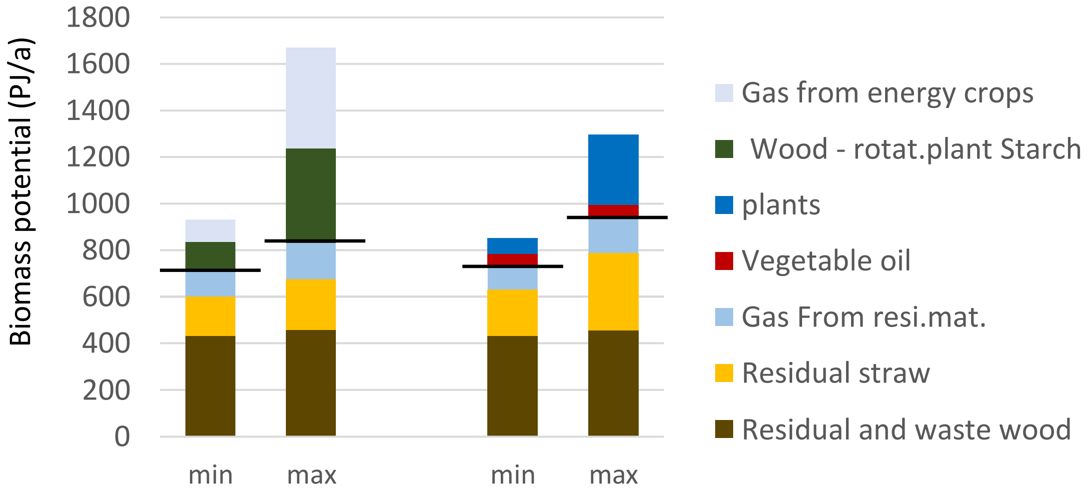


Figure 13 Biomass potential in Germany in 2050 (according to [30])

With the hitherto unused and thus available potential of about 930 PJ, about 8.5 million tons of GHG-reduced fuels could be produced - **without** considering competing uses. This would correspond to about a quarter of the current demand for diesel fuel or about 60% of the demand for light heating oil. Approximately 35 million metric tons of CO2 equivalents could be saved, corresponding to 20% of transportation-related and 4% of total GHG emissions in 2019.



with energy crop cultivation with RME/EtOH (1G)

Figure 14 Biomass potential in Germany as a function of the plant species used (according to [31]).

Figure 14 shows the results of an estimate from 2009 for different cultivated areas (minimum: 1.8 million ha, maximum: 4.0 million ha). It can be seen that the biomass potential also depends on the respective type of use. For energy use, fast-growing and fully usable energy crops achieve the higher yields compared to biomass for conventional biofuels from fats or starch or sugar [31], [15].

Regardless of this, however, it must be stated that the German energy demand cannot be covered by domestic biomass by far. The potential is also insufficient for the transport sector, even if given competing uses are not considered and it is assumed that the available biomass is used entirely for the production of fuels and not, as is the case today, predominantly for the provision of heat and electricity.

A report [32] prepared by the JRC on behalf of the European Commission provides data differentiated by country on the development of the biomass potential that can be used for energy purposes until 2050. Different scenarios are considered, which differ in various basic assumptions. One major difference is the degree of non-energy use of the biomasses covered, which can be up to 90% for the minimum scenario. In addition to energy crops (e.g., cereals, sugar beets, oil crops, miscanthus), agricultural residues (e.g., manure, straw), fuelwood, and forestry residues, organic waste (including household waste, sewage sludge) was included. The results for 2050 are summarized in Figure 15.

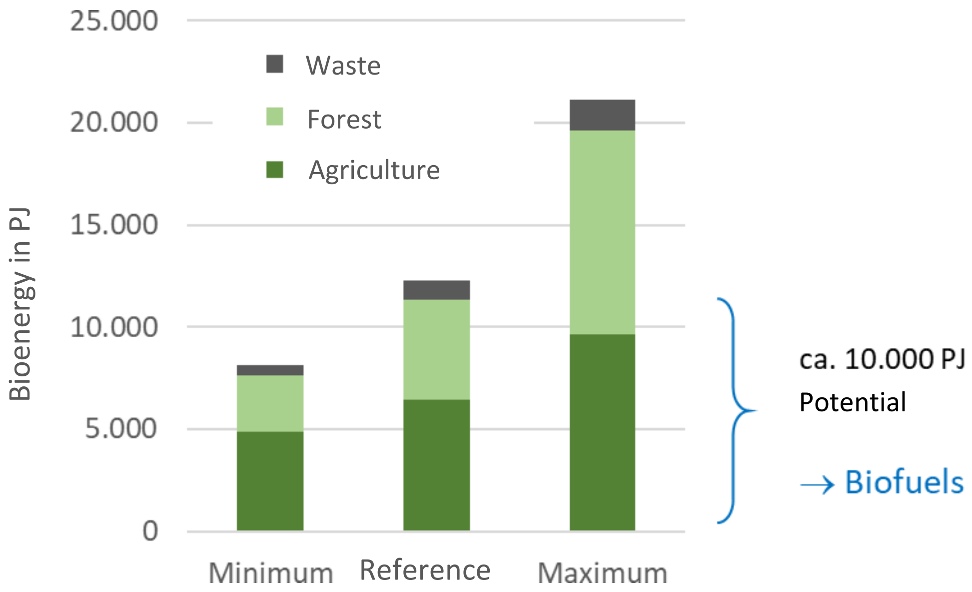


Figure 15 Forecast of biomass potential in the EU 28 (2050), according to [32]

For Germany, the reference case shows a potential of 1,440 PJ and, with high availability, 2,565 PJ. The FNR estimate of 1,800 PJ is therefore somewhere in between. Other studies estimate the European biomass potential for 2030 at around 15,000 PJ. This value also lies between the reference and maximum scenario of the JRC report (see Figure 15).

Bioenergy is increasingly traded across Europe and globally. In a conceivable distribution model, the total potential could be broken down according to the population of the member countries. Assuming a biomass potential of 10,000 PJ available for fuel production in Europe, Germany, with a population share of 16%, would account for about 1,600 PJ annually (corresponding to about 15 million tons of biofuels).

Sustainability and acceptance

The cultivation of energy crops is discussed very controversially, not only in Germany. The reasons for this are:

- the possibly ethically unjustifiable use of food and feed or corresponding arable land for energy production ("plate or tank" discussion),
- the possibly ethically unjustifiable use of food and feed or corresponding arable land for energy production ("plate or tank" discussion),
- negative impacts of energy crop cultivation on nature and the environment.

This is countered by the possibility of sustainable extraction of energy raw materials as a positive aspect. In this context, the Federal Environment Agency divides the fuels that can be produced from biomasses into different generations according to the type of raw materials used and is guided by the criteria of sustainability (Table 4) [33].

Table 4 Biofuels - Definition of generations [33]

Generation	Raw material	Product (Example)
1. Generation	Growing biomasses (e.g., cereals, oil plants, sugar beets)	Biodiesel, bioethanol Hydrogenated vegetable oil
2. Generation	Biomasses without competition for use with food (e.g., residual wood, straw, green waste, waste biomass).	Cellulosic ethanol, synthetic fuels (BtL, bio SNG)
3. Generation	Biomasses that can be obtained independently of crops (e.g., algae).	Algae biodiesel, algae ethanol

The alternative fuels currently in use are predominantly conventional 1st generation biofuels, the use of which has been criticized for the reasons mentioned above. In Germany, these products were counted at a maximum of 6.5% of energy consumption in the transport sector for the fulfillment of the obligation to reduce GHG emissions [34]. The revised version of the 38th BImSchV provides for a further reduction of the cap to 4.4%. In contrast, 2nd and 3rd generation fuels are considered advanced biogenic fuels for which minimum shares are required in 2030 (see Table 2).

With the introduction of the Renewable Energy Sources Act (EEG) and the purchase obligation and feed-in tariff enshrined therein in 2000, the cultivation of especially silage or green corn as the most favorable substrate for biogas plants from an economic point of view has grown very strongly. This trend has been associated with the negative effects of energy crop cultivation under the term "cornification" [35], [36]. Especially the permanent cultivation of only one species (monoculture) can lead to humus loss, soil erosion as well as to an increased input of pollutants into the soil (pesticides and fertilizers). The amendment of the EEG in 2012 has resulted in the absence of an unrestrained increase in corn cultivation. Since then, the area used for corn cultivation (approximately 2.5 million hectares) has remained almost constant. In 2019, 1.7 million hectares of feed corn and 1.0 million hectares of corn for biogas plants and electricity generation were cultivated in Germany [29]. The latter corresponds to a 6% share of agricultural land. Due to its high GHG mitigation potential, corn was the main raw material for the production of bioethanol as a substitute for gasoline in Germany in 2018, with a share of 50%. However, only 1.6% of the grain corn required here comes from domestic production [37]. Therefore, there is currently no basis for a "cornification debate" in Germany.

Nevertheless, it should be noted that, from an agricultural point of view, rapeseed cultivation plays an essential role in crop rotation with cereals. Thus, the winter wheat yield increases by about 10% compared to cultivation without crop rotation [38]. At the same time, the production of biodiesel from rapeseed oil produces important and high-quality co-products in the form of extraction and pressing residues. Rapeseed meal is the most important source of protein in Germany [38].

Present situation

Germany has 16.7 million hectares of agricultural land. This corresponds to slightly less than half of the total area. A further third is covered by forests, while the remainder is made up of settlement, transport, and water areas (Figure 16) [29]. In 2019, energy crops were grown on about 14% of the agricultural land, mainly for biogas production. Less than 5% of arable land was used for liquid biofuel production [39].

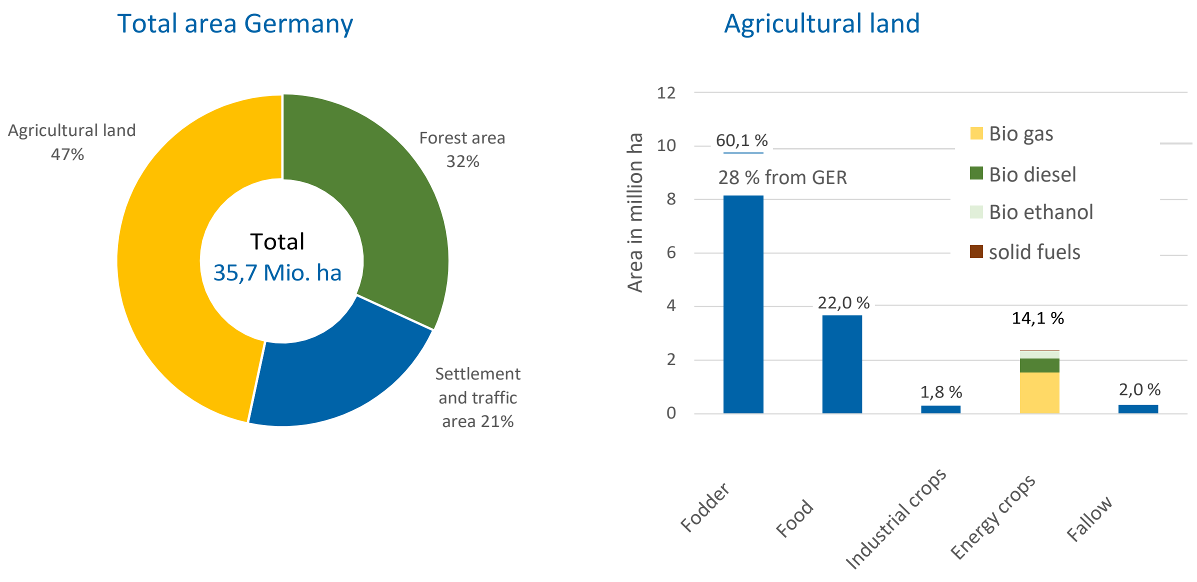


Figure 16 Land use in Germany 2019 according to [29]

Following the discontinuation of tax incentives for biofuels in 2007, quotas or, from 2015, GHG reduction targets have served as a driver for their application. As a result, the amount of biofuels brought to market decreased from 4.6 to 3.4 million tons in 2019, which was associated with a decrease in the biofuel share of total fuel consumption from 7.5% to 4.7% (energetic) [5], [39].

In 2019, nearly 125 PJ of biofuels, mainly as blends in the form of biodiesel (FAME) and bioethanol, were placed on the market in Germany (see Figure 17) [40]. This reduced GHG emissions by 9.5 million t CO2, eq. However, a considerable part of the raw materials for biofuels does not originate from Germany.

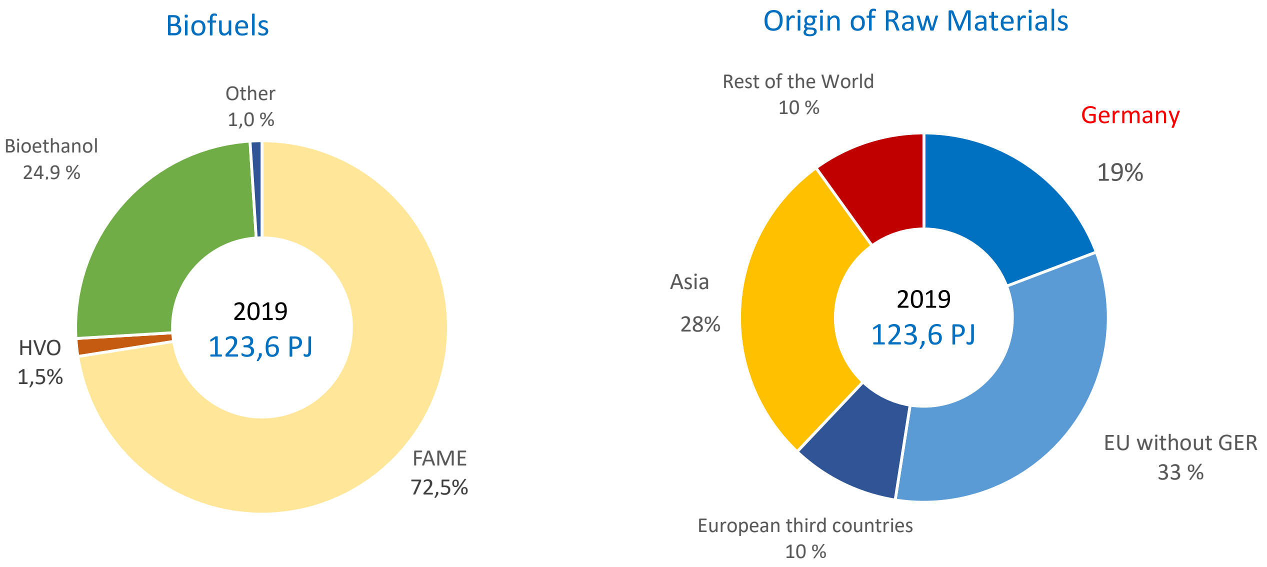


Figure 17 Biofuels by fuel type, D 2018 [40]

As shown in Figures 18 and 19, this mainly concerns palm oil and sugar cane imported from Asia and South America, respectively. However, corn used for bioethanol production and used cooking oil (UCO), which has become the most important FAME feedstock, are also mainly imported [40].

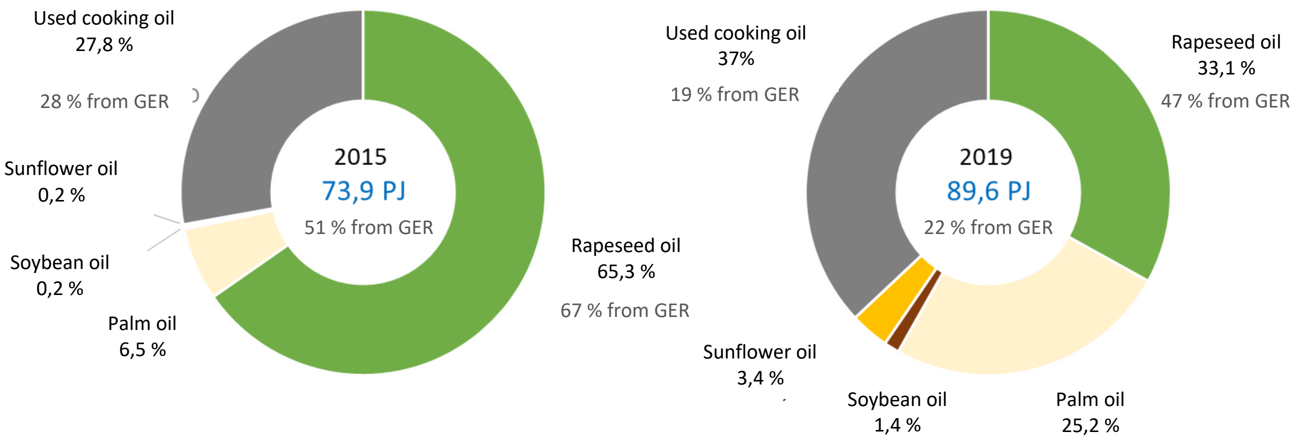


Figure 18 Raw materials for FAME, D 2015 and 2019 [40]

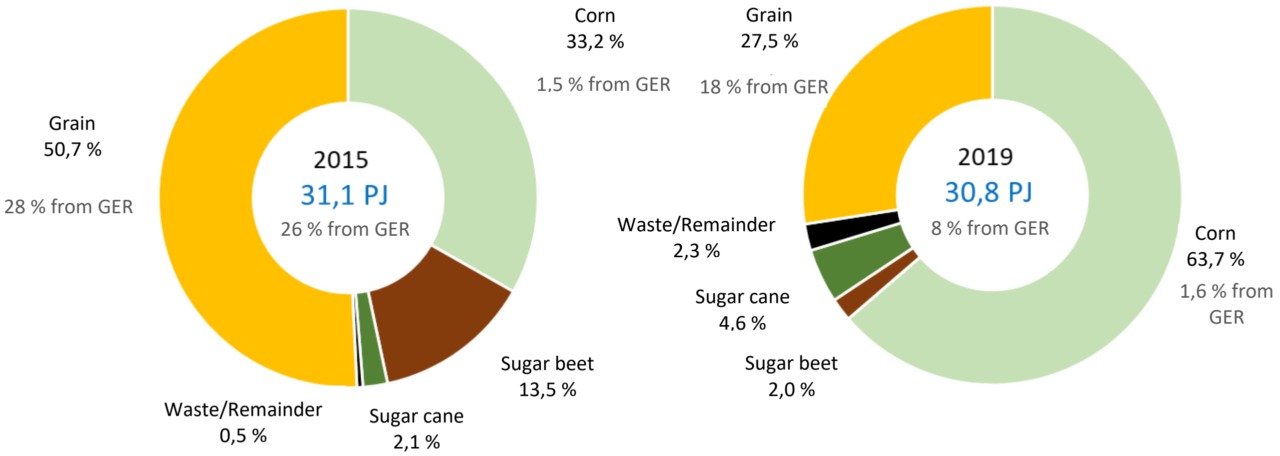


Figure 19 Raw materials for bioethanol, D 2015 and 2019 [40]

In 2015, the quota regulation practiced until then in Germany regarding the use of alternative energy sources in transport was replaced by an obligation to reduce greenhouse gases through the fuels placed on the market (BImSchG). As a result, there has been a significant shift in the feedstock base in favor of biomasses with a low GHG footprint. For example, the use of corn has increased sharply, while sugar beets have become less important as a feedstock for ethanol production despite high yields per hectare. Of particular interest are waste and residual biomasses, which per se have a low GHG footprint. Used cooking oils have thus replaced rapeseed oil as the main feedstock for biodiesel production in 2016 [37].

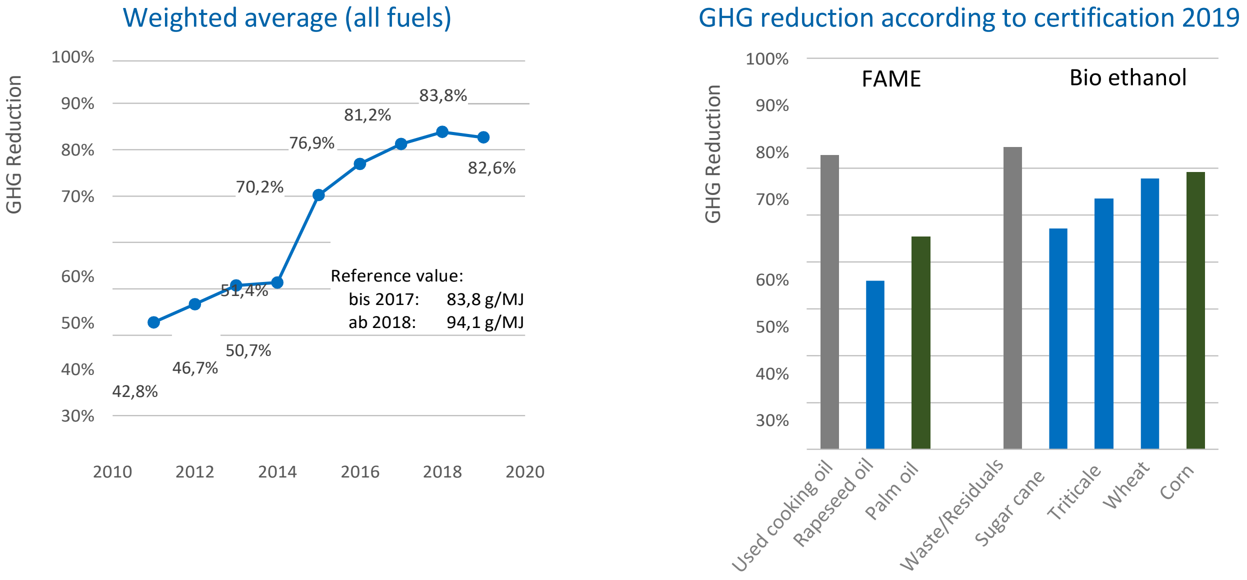


Figure 20 Development of GHG reduction of biofuels compared to fossil reference, D (data source: [40]).

Supported by measures to improve efficiency and sustainability throughout the biofuel production chain, their GHG footprint decreased from an average of 40.75 g CO2 equivalent per MJ (2014) to 16.37 g CO2 equivalent per MJ (2018). In relation to the reference values for fossil fuels, this means reductions in the specific GHG emissions of 51.4% (2014) and 82.6%

(2019), respectively (Figure 20) [37]. As a result, the emission reduction required by the legislator can be achieved with lower biofuel shares.

Biofuels produced from waste or residual biomasses are not subject to the restrictions introduced for 1st generation fuels. However, it should be noted that fuel standardization specifies upper limits for FAME or ethanol, which must be adhered to regardless of the feedstocks used [41], [42].

To produce biodiesel (fatty acid methyl ester) from wastes and residues, industrial waste fatty acids and animal fats can be used in addition to used cooking oils, according to Annex IX, Part B of RED II. Figure 21 shows the results of the Mittelstandsverband abfallbasierter Kraftstoffe e. V. for estimating the raw material potentials [43] for Germany and Europe. The comparison with biodiesel consumption in Germany makes the limited supply very clear. In this context, it should be noted that the quota system for GHG reduction already practiced in Germany since 2015 will be binding throughout the EU as of 2020, so that demand for such feedstocks will increase dramatically outside Germany.

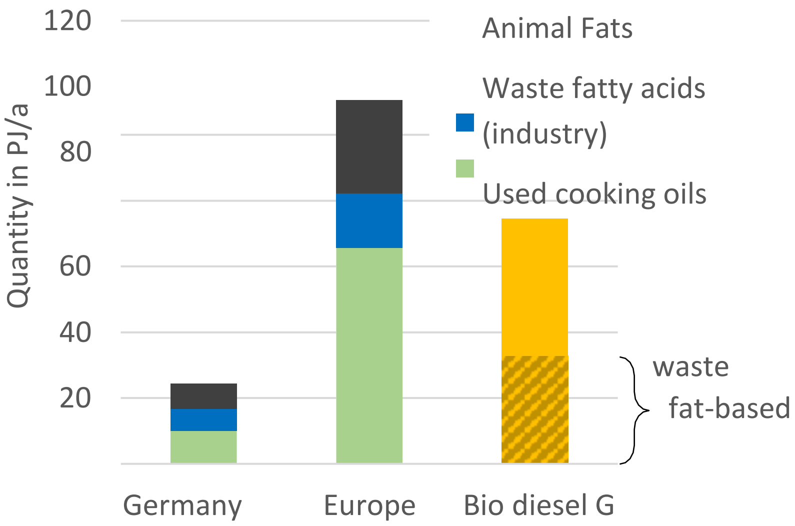


Figure 21 Potential for waste fat-based biofuels compared to the amount of biodiesel currently used [43].

2.3. Carbon dioxide

The greenhouse gas carbon dioxide (CO2) in itself can be considered as a carbon source. In the natural process of photosynthesis, atmospheric CO2 serves to build complex organic compounds (biomass), which can also be available for energy use (see section 2.2.). But also industrially, hydrocarbon-based fuels can be synthesized by a reaction with hydrogen.

Atmospheric carbon dioxide

Carbon dioxide is one of the trace gases contained in the earth's atmosphere. The concentration was 280 ppmv pre-industrially and has increased to about 410 ppmv currently, mainly because of the combustion of fossil fuels. The carbon inventory of the atmosphere is currently about 850 gigatons. The potential for producing energy sources is virtually unlimited, especially since they are oxidized back to carbon dioxide and water when used (closed carbon cycles). The atmosphere contains 0.001 % of the total carbon available on earth. At more than

99.9 %, the lithosphere is where the bulk of it is stored in the long term.

In principle, it is technically possible to filter carbon dioxide out of the atmosphere (DAC: Direct Air Capture) and feed it concentrated for further use. However, separation is very complex due to the extremely low CO2 concentration. Conventional physical scrubbing is unsuitable for this purpose, and extraordinarily large volumes of air must be moved and treated (more than 1.3 million m^3 of air per ton of CO2). This entails correspondingly large plant technology and high energy expenditures (fans, regeneration of filters).

Point sources

Carbon dioxide is formed in many industrial plants and is released into the atmosphere with the exhaust gas in sometimes very high concentrations. In addition to fossil-fired power plants, steel mills, cement plants and chemical industry plants, these also include biogenic sources such as processing plants for biogas or ethanol plants. The high CO2 contents allow the use of classical and technically introduced gas separation processes, resulting in significantly lower CO2 costs compared to capture from air. In some cases, CO2 capture is already part of the existing plant due to the technology (e.g., ammonia synthesis), so that no additional expenditures are necessary. Table 5 gives an overview of possible sources and typical CO2 contents. The quantities listed are mostly the CO2 emissions covered by emissions trading; they are not to be equated with possible potentials. The figures for the production of bioethanol and biomethane are based on our own calculations. In total, the amount of CO2 would theoretically enable the production of more than 100 million metric tons per year of synthetic fuels.

Table 5 GHG emissions in Germany (2019) [44]

CO_2-Source	**Emissions in Mio. t/a**	**typical CO2 levels**
Public power plants	219,0	9-15 Vol.-%
Refineries	23,2	3-13 Vol.-%
Cement industry	20,0	14-33 Vol.-%
Chemical industry (ammonia synthesis)	4,4	>99 Vol.-%
Steel and iron metallurgy	35,6	18 Vol.-%
Aluminum	1,0	
Bioethanol*)	0,6	>99 Vol.-%
Biogas (upgrading to biomethane*)	1,0	>99 Vol.-%
Combustion biomass (biogas, solid biomass)	48,5	12-17 Vol.-%
Total	351,6	

*) own estimate

Most of the carbon dioxide emitted comes from the combustion of fossil fuels to generate electricity and heat. The lignite-fired power plants Neurath, Boxberg, Niederaussem, Jänschwalde, Weisweiler and Schwarze Pumpe are the largest CO2 point sources in Germany with annual emissions between 8.9 and 22.6 million tons (2019) [44]. Due to the increasing use of renewable energy, the CO2 emission factor in the electricity mix (generation) has already decreased significantly from 764 to 401 g CO2/kWh since 1990 (-48%). Correspondingly, with increased electricity generation, annual CO2 emissions have fallen in absolute terms from 366 to 219 million tons (-40 %) [45]. In the course of the energy transition, GHG emissions in this sector will continue to decrease sharply.

Another part is also formed from fossil carbon, but is produced as a reaction-related by-product of chemical conversion (e.g. during the reduction of iron ores or the generation of synthesis gas for ammonia synthesis). Ammonia and methanol are among the most important basic chemicals, with global production of 200 and 150 million metric tons per year, respectively. About 90% of ammonia is used to produce nitrogen fertilizers, while methanol is increasingly used for the production of primary and platform chemicals (C1-Chemicals), with a strong upward trend. The synthesis gas required for production (N2/H2 mixtures, CO/H2 mixtures) is currently obtained almost exclusively from natural gas or coal. In the case of ammonia synthesis in particular, the carbon introduced with the raw material must be converted into carbon dioxide and separated by gas scrubbing. During the regeneration of the scrubbing agent, carbon dioxide is produced in pure form and is currently partially released into the atmosphere. In principle, this CO2 would be available - at least in the medium term - as a low-cost raw material source for the synthesis of fuels. In the long term, it is conceivable that fossil hydrogen could be replaced by electrolytically produced hydrogen, which would eliminate this CO2 source.

In the burning process to produce cement clinker, the so-called deacidification of the limestone leads to the release of carbon dioxide. While the energy-related GHG emissions can be avoided by using renewable energy, the amount of process-related carbon dioxide can practically only be reduced by reducing the use of cement clinker or lime in the building materials industry. In the long term, a "CO2 base load" of about 9 million t/a is expected in Germany, which from today's point of view could only be avoided by permanent storage (CCS) [46].

On the way to the greatest possible greenhouse gas neutrality after 2050, CO2 emissions in industrial waste gases and thus also the CO2 potential available for the production of synthetic fuels will gradually decrease in line with environmental policy targets and scientific and technical progress. Table 6 summarizes forecasts of the amounts of CO2 available in point sources in the future [46], [47]. It can be seen that even in an ambitious reduction scenario, considerable quantities of CO2 will still be available in 2050. These will then largely come from the combustion of biomass and waste. However, it should be noted that the very low emissions in the cement clinker and limestone industry, the chemical industry or metallurgy shown in the studies can only be achieved by CCS. The residual CO2 produced in these sectors can also be considered as potential feedstocks for the synthesis of fuels.

Table 6 CO2 potential Germany (important point sources) [46], [47]

Emissions in Mio. t CO_2	**80 % Scenario**			**95 % Scenario**		
	2020	**2030**	**2050**	**2020**	**2030**	**2050**
Public and industrial power plants	230,4	167,8	38,7	192,9	94,5	9,7
Refineries (refinery gas)	7,2	5,2	1,5	7,3	5,3	0,7
Cement industry	12,0	11,0	9,4	11,4	8,1	0,4
Chemical industry (NH3 synthesis)	7,5	7,5	7,5	7,5	6,0	0,4
Steel and iron metallurgy	15,2	12,2	7,2	17,0	10,8	0,4
Aluminum	0,6	0,5	0,4	0,6	0,5	0,4
Biomass combustion (heat, power)	48,5	28,8	21,4	36,2	28,2	19,1
Biomass combustion (process heat)	7,3	19,0	42,5	12,2	28,0	35,9
Total	326,7	249,7	128,6	281,2	178,4	66,5
Fuel potential (e-fuels) in Mill. t *)	105	80	41	90	47	21

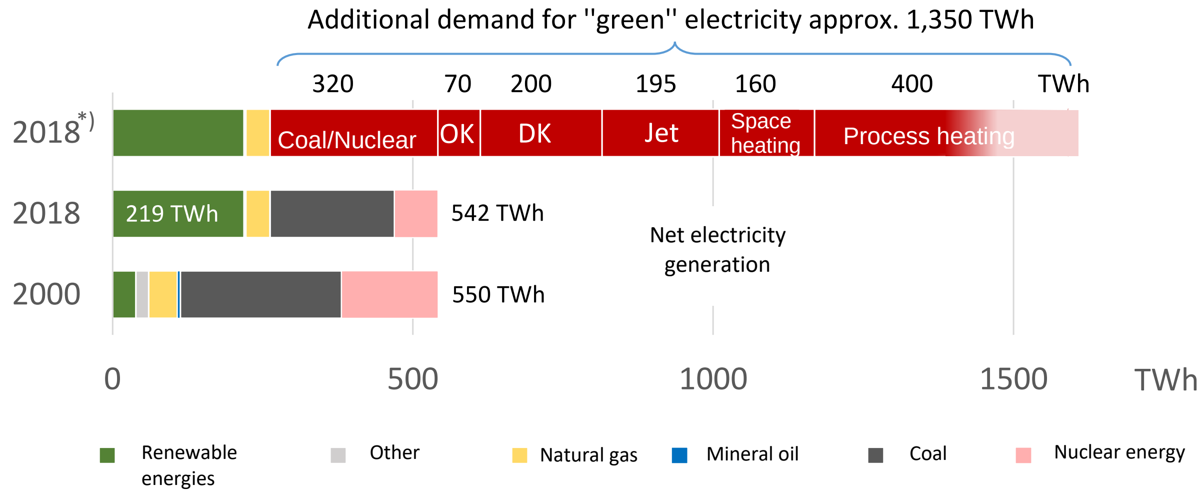
*) via PtL: approx. 0.32 kg fuel per kg CO2 (theoretically with complete capture)

In these cases, however, the carbon cycles are not closed. This is a multiple use of carbon dioxide, which does not reduce absolute emissions. In the transport sector, however, no additional emissions are generated either. When considered integrally, the use of CO2 point sources of fossil origin also leads to a reduction in GHG emissions. Regarding the targeted GHG-neutral economy in the 2nd half of this century, however, only biogenic carbon dioxide is available as an alternative to "direct air capture" in the long term. However, as long as carbon dioxide is still released into the atmosphere from point sources in relevant quantities, capture from the atmosphere does not make sense from both technical-economic and environmental perspectives. The development and market introduction of technologies to produce CO2-based energy carriers can be significantly facilitated and promoted by the use of comparatively inexpensive point sources during a transitional period. This applies in particular to industrial sites in Europe.

2.4. Electric Energy

Electricity demand

The use of renewable energy sources is essential for greenhouse gas-neutral heat supply and mobility. A central role will be played here - in addition to the "direct use of renewable energies in the respective sectors" [2] - the electrification of all relevant areas will play a central role. "In the transport sector, this will succeed both through the introduction and spread of direct electric drive technologies and - in perspective - using electricity-based fuels" [2] and "in the building sector, electricity from renewable energies (...) plays an increasingly important role in heat supply" [2]. Figure 22 illustrates the dimension of these ambitious goals. In 2016, net electricity generation amounted to 615 TWh [48], [49], of which about one third was produced from renewable energy sources. The additional electricity required for the complete conversion of road transport to electric drives is thus slightly more than 270 TWh. This value is based on domestic consumption of DK and OC in 2016 and tank-to-wheel efficiencies for internal combustion engines and electric drives, respectively. A further 195 TWh would be required for the synthesis of jet fuel from carbon dioxide and electrolysis hydrogen (for calculation basis, see Annex 8).



*) Estimated electricity demand with full electrification of the transport and heat sectors

Figure 22 Net electricity generation (D, 2018) and additional demand for mobility and heat [3]

The inclusion of the heating market (space and process heating, hot water, cooling) leads to a further increase in the demand for "green" electricity. In 2015, final energy of 1,373 TWh was consumed in Germany for the provision of heating and cooling. Deducting the contributions of electricity and renewable energy sources, a residual demand of about 1,050 TWh remains, which will have to be reduced in the future by increasing efficiency and eventually covered by electrical energy during sector coupling [50]. Assuming that heat pumps (coefficient of performance 4) will be used in the future to provide space heating and hot water, this results in an additional electricity demand of about 160 TWh. The demand for process heat and cooling amounts to 420 TWh (for calculation basis, see Annex 8). Future savings to be expected from better insulation and efficiencies were not considered. In addition, the phase-out of nuclear energy and coal requires the substitution of 320 TWh.

Based on current energy consumption, full electrification of the transportation and heating sectors results in a total electricity demand of 1,300 to 1,500 TWh. This is currently offset by approximately 250 TWh of electricity from renewable energy.

Power generation

Gross electricity generation in Germany amounted to 610.2 TWh in 2019. Almost 44% of this was generated in thermal power plants from fossil fuels, including 28% in coal-fired power plants [51]. Thus, for the first time, more electricity was produced in Germany from renewable sources than from lignite and hard coal combined. In 2020, electricity generation dropped to 572 TWh - probably also due to the Corona pandemic. (see Figure 23 Gross electricity generation in Germany (2020)), but at the same time the absolute amount of renewable electricity grew from 243 to 251 TWh [50].

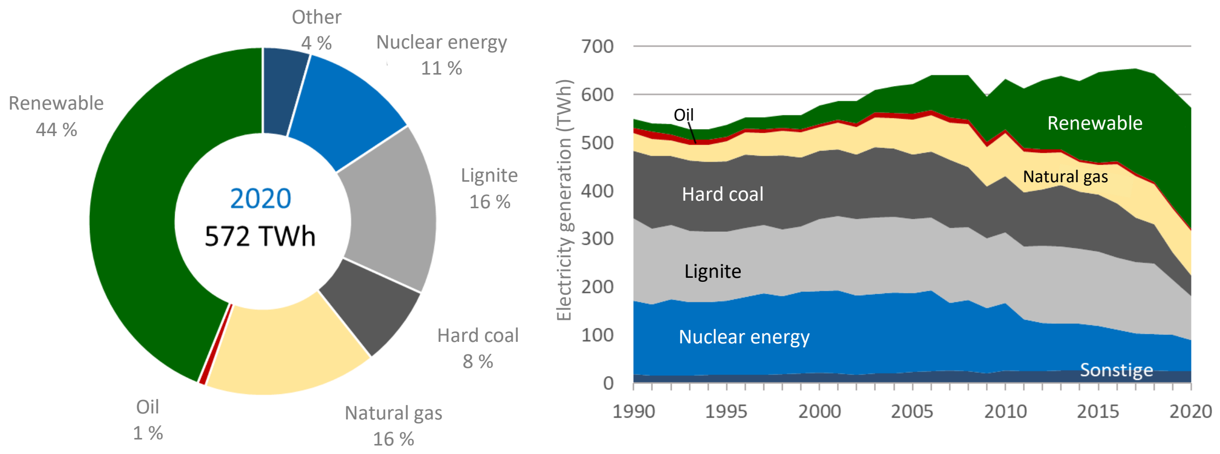


Figure 23 Gross electricity generation in Germany (2020), data source [50]

The generation of electricity from renewable sources cannot be demand-driven. For wind and solar power in particular, generation is highly dependent on the weather. Periods in which only little renewable electricity can be produced (so-called "dark lulls") are contrasted by phases with a lot of wind and sun. On the one hand, generation capacities must be kept available to meet demand regardless of external circumstances; on the other hand, wind power plants in particular must be temporarily shut down if the supply is too high. To balance out differences between electricity supply and demand, electricity is exchanged across national borders. With the increasing expansion of renewable energy in Germany, it can be observed in recent years that more electricity has been exported than imported and that the GHG footprint of imported electricity continues to be higher than that of exported electricity. This results in a higher specific emission value of 427 g/kWh for electricity consumed domestically (electricity mix) than 401 g/kWh for domestic generation.

Development of electricity generation from renewable sources

Various studies have dealt with the forecast of the amount of electricity that can be produced from renewable sources in Germany in the future. Technical developments in plant technology play just as important a role as the expansion of offshore wind power plants, social acceptance, or the economic and political framework conditions.

Figure 24 shows the results in comparison to today's status (2019) [10], [12], [52]. Both for the installed capacity (left figure) and derived from this for the electricity generation (right figure), the studies show comparable results. Thus, an installed capacity for renewable electricity generation of around 200 GW is expected in the future in the final expansion. This is in line with the expansion target of the German government [52]. With this value, an electricity generation between 450 and 500 TWh/a can be expected. This is about 2 times the current production. An exception is the electrification scenario of the German Energy Agency dena, which primarily assumes a significantly higher onshore wind supply in its consideration in scenario EL95.

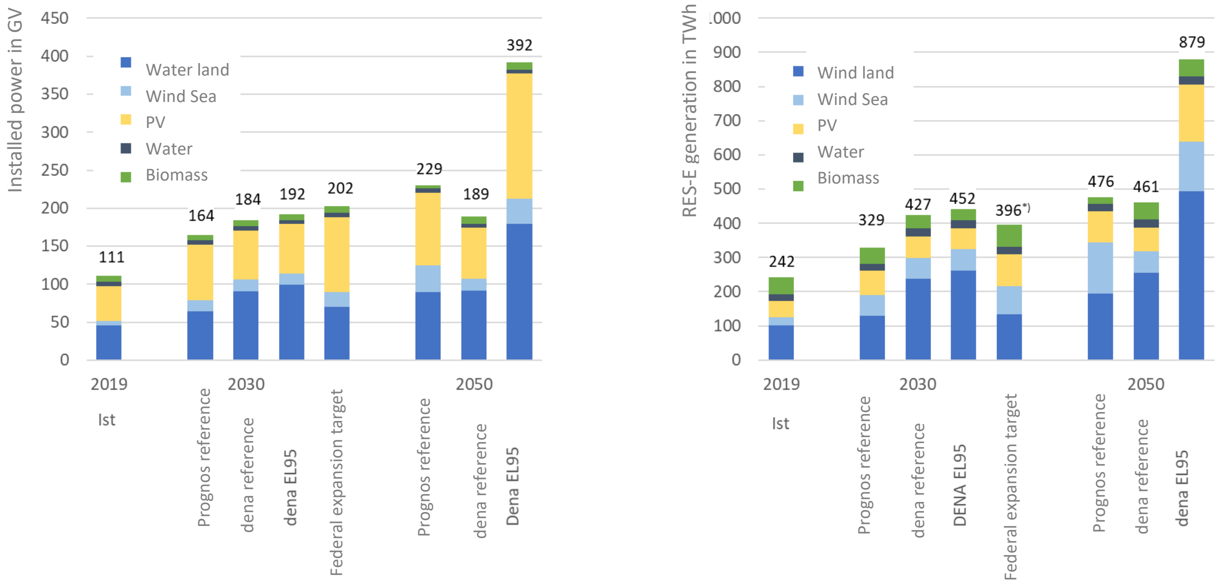


Abbildung 24 Forecast of Installed Power Plant Capacity (left) and Electricity Generation (right) from Renewable Sources [10], [12], [52]

International comparison

Table 7 shows a comparison of installed power plant capacities based on renewable energy sources for the world, the EU28 and Germany, broken down by primary energy source [5]. In addition, important key figures are compiled.

Relative to population size, Germany and Europe contribute somewhat disproportionately to both primary energy consumption (PEV) and CO2 emissions. However, the shares of power plant capacity (renewable) are considerably larger than the respective population shares. This is also true for electricity generation in 2019 (Table 8).

Table 7 Installed power plant capacity (2019) [5]

	Installed capacity (GJ)			**Share**		
	World	**EU28**	**G**	**EU/World**	**G/World**	**G/EU**
Generation ges. Renewable generation	2.588	467,0	125,5	18,0%	4,8%	26,9%
Share RE						
Wind	651	179,1	60,8	27,5%	9,3%	33,9%
PV	627	114,7	49,0	18,3%	7,8%	42,7%
Hydro	1.150	130,8	5,6	11,4%	0,5%	4,3%
Biomass	139	39,0	10,0	28,1%	7,2%	25,6%
Other	21	3,4	0,048	16,2%	0,2%	1,4%

	Welt	EU28	D	EU/Welt	D/Welt	D/EU
Population (bn)	7,63	0,51	0,08	6,7%	1,1%	15,6%
CO2 emissions (Gt)	34,2	3,3	0,684	9,6%	2,0%	20,7%
PEV (PJ)	583.900	68.810	13.140	11,8%	2,3%	19,1%

Table 8 Power generation (2019) [5]

	Generation TWh			**Share**		
	World	**EU28**	**G**	**EU/World**	**G/World**	**G/EU**
Generation ges.	27.011	3.272,2	610	12,1%	2,2%	18,4%
Renewable generation	7374	1.079,4	242,5	14,6%	3,3%	22,5%
Share RE	27,3%	33,0%	39,8%			
Wind	1.594	377,8	125,9	23,7%	7,9%	33,3%
PV	756	123,1	46,4	16,3%	6,1%	37,7%
Hydro	4.295	378,9	20,1	8,8%	0,5%	5,3%
Biomass	594	188,9	50,0	31,8%	8,4%	26,5%
Other	135	10,8	0,2	8,0%	0,1%	1,9%

On a global scale, electricity generation from hydropower is by far the first renewable primary energy source. In contrast, the average in the European Union relies on wind and biomass. In addition, photovoltaics in particular play a prominent role in Germany, despite the comparatively unfavorable climatic conditions.

Table 9 Renewable Power generation of selected countries (2018) [5]

2018	**RE-Energy (total)**	**Share EU28**
Germany	230,9 TWh	21,4%
France	118,7 TWh	11,0%
Italy	116,1 TWh	10,8%
UK	110,6 TWh	10,2%
Spain	106,4 TWh	9,9%

Table 9 shows the renewable electricity generation of selected countries. With a share of 21.4 %, Germany is by far the largest European producer of e-electricity. The German share of installed capacity is even higher (wind 34 %, PV 43 %). Against this background, it is questionable whether Germany will be able to cover demand gaps in the medium term through imports from other European countries.

2.5. Hydrogen

Hydrogen is a key component in the energy and chemical sectors and finds its application in a wide variety of forms:

- as a fuel (direct combustion, feed into the natural gas grid),
- as a fuel (energy source for fuel cells, H2 engines),
- as a raw material to produce synthetic fuels ("BtL", "PtL"),
- as an "auxiliary material" for hydrogenation processes in petroleum refineries or the chemical industry.

Its importance will grow strongly in the future against the background of the required reduction of greenhouse gas (GHG) emissions.

Currently, the conversion of natural gas through a process known as steam reforming is the most cost-effective way to produce hydrogen and is thus the preferred way to meet demand ("gray" hydrogen).

Hydrogen can also be produced by electrolysis of water. If electricity generated from renewable sources is used, GHG emissions can be largely avoided ("green" hydrogen). However, hydrogen can also be produced from fossil natural gas with a greatly reduced GHG footprint. To do this, the carbon chemically bound in the natural gas must be captured and permanently deposited. In the case of steam reforming as well as the related autothermal reforming, the carbon is produced in the form of carbon dioxide. This can be captured and stored in geologically suitable formations (carbon capture and storage, CCS). If hydrogen plants are coupled with CCS, the current discussion refers to "blue" hydrogen. In the process of natural gas pyrolysis, on the other hand, the hydrocarbons contained (predominantly methane) are broken down into the elements hydrogen and carbon. The latter could be separated as a solid and deposited ("turquoise" hydrogen).

2.6. Interim conclusion

Biomass

Biomass is an important renewable raw material source for a sustainable energy industry. Germany has a high potential of energetically usable biomass. However, considering expected competing uses (heat supply, power generation, material use), it will not be sufficient to meet the demand for advanced fuels in the long term.

The potential estimates for the European Union show considerable regional differences, but also indicate a very large overall potential. When divided up according to population size, it appears possible for Germany to meet its demand for fuels.

In contrast, the German and European potential of biowaste for the production of FAME/HVO ("used cooking oils") is very limited.

Carbon dioxide

Carbon dioxide as a component of the atmosphere is available in practically unlimited quantities. However, due to its very low concentration, capture and extraction is very energy-intensive and requires very large production plants. This leads to a massive increase in production costs (see section 3.4.2).

At present, enormous amounts of carbon dioxide are emitted with industrial waste gases. Separation is much easier, since the CO2 concentrations are usually in the 2-digit percentage range and in some cases are even close to 100 %. Even if society is largely "defossilized" after 2050, the potential of CO2 point sources is sufficient to produce around 20 million tons of e-fuels. The carbon dioxide would then come predominantly from biomass use for the provision of building and process heat.

e-Electricity

Both global and regional demand for electricity from renewable sources will increase dramatically in the future. The causes are the growing electrification of all areas of society in the course of the energy transition, but also the move away from electricity generation from coal and nuclear power. Based on today's energy consumption, the demand for Germany has been estimated at approximately 1,300 TWh.

In view of the climatic and geographic boundary conditions, the expansion possibilities for renewable power generation are limited. The generation that can realistically be achieved in the future is about 500 TWh. Currently, most of the energy required in Germany is imported. This will also be necessary in the future.

With a share of 21.4%, Germany is by far the largest European producer of e-electricity. The German share of installed capacity is even higher (wind 34 %, PV 43 %). Against this background, it is questionable whether the demand gaps can be covered by imports from other European countries in the intermediate term.

3. Possibilities for the production of GHG-reduced fuels.

3.1. Overview

To produce hydrocarbon-based fuels for internal combustion engines and aircraft turbines as well as liquid fuels, all carbon-containing raw materials can be considered in principle. In addition to biomasses as renewable carbon carriers, electricity generated from renewable sources together with carbon dioxide can play a significant role in sustainable power and fuel production. Figure 25 provides an overview of the different raw material classes and the possibilities for obtaining liquid fuels.

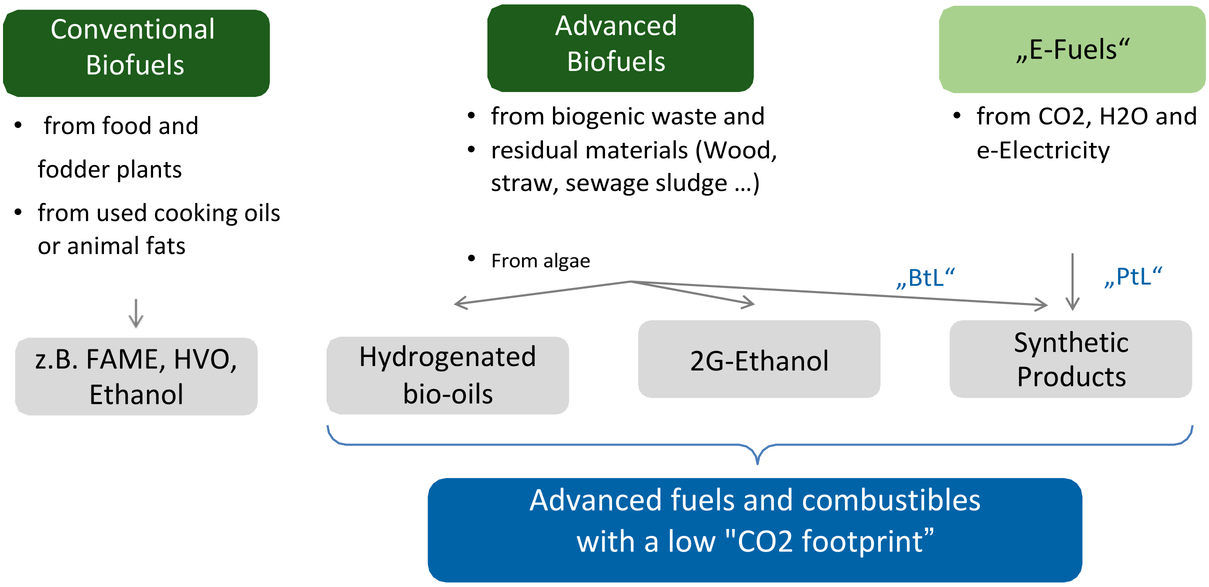


Figure 25 Raw materials and processing possibilities

For example, carbohydrates such as sugar, starch or cellulose can be degraded by fermentation to ethanol and higher alcohols, ketones, or even aliphatic hydrocarbons. These are suitable as substitutes for fuels, either directly or, if necessary, after chemical upgrading. Feedstocks are sugar- and starch-containing plants as well as lignocellulose (wood, straw). Oil plants as well as various types of algae contain lipids that can be separated and relatively easily converted into fuels. Any organic feedstock can be converted into biogenic oils by direct liquefaction. As a rule, multi-component mixtures with high oxygen and nitrogen contents are obtained, which require complex processing by hydrogenation. The production of synthesis gas (CO/H2 mixtures) by gasification does not place high demands on the chemical composition of the starting materials, so that lignocellulose or undefined biomasses can also be considered as raw materials. Synthesis gases can also be produced independently of biomass based on carbon dioxide and water using electrical energy. Via various syntheses (e.g. Fischer-Tropsch synthesis, methanol synthesis), the gases can be converted into high-quality liquid energy carriers. Such process chains are referred to as biomass-to-liquid or power-to-liquid processes (BtL, PtL).

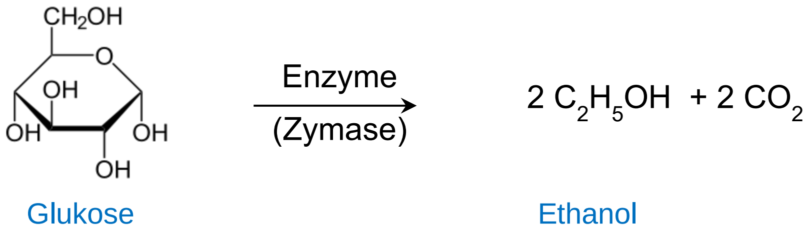
In the following sections, the individual process chains are briefly presented. A detailed description can be found in [3].

3.2. Conventional biofuels

3.2.1. 1G-Ethanol

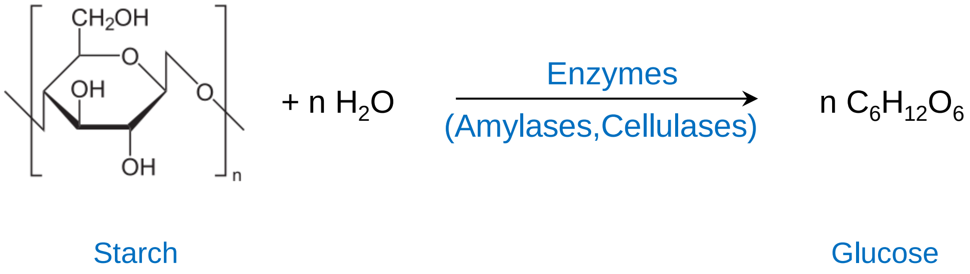
Ethanol has been known as a suitable fuel practically since the invention of the gasoline engine (spirit -> "fuel") and can be obtained from sugars (sucrose, glucose) via classical alcoholic fermentation according to equation (1).

(1)



$$\xrightarrow[\text{(Zymase)}]{\text{Enzyme}} 2\,C_2H_5OH + 2\,CO_2$$

If plants that could also be used for feed or food production (e.g. sugar beet, wheat, corn) are used to obtain starch, the product is referred to as 1st generation bioethanol (1G ethanol). When complex carbohydrates (e.g., starches) are used, enzymatic breakdown of the polysaccharides to disaccharides (sugars) is required prior to fermentation (equation (2)).



$$+\, n\,H_2O \xrightarrow[\text{(Amylases,Cellulases)}]{\text{Enzymes}} n\,C_6H_{12}O_6$$

The production of bioethanol also for the purpose of energy use is a technology that has been introduced on the market. A simplified process diagram is shown in Figure 28. Table 10 summarizes important key data to produce 1st generation bioethanol.

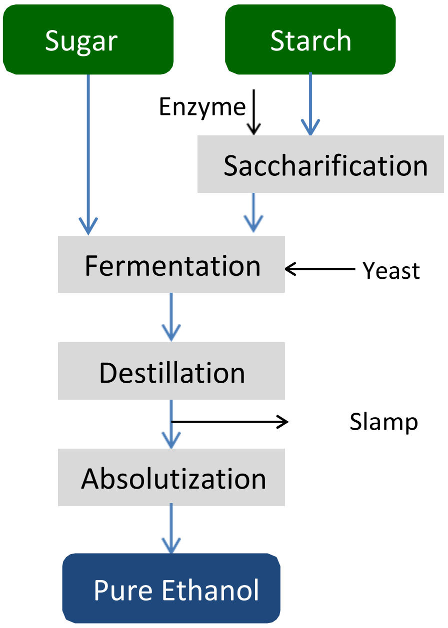


Figure 26 Process diagram production of 1st generation bioethanol

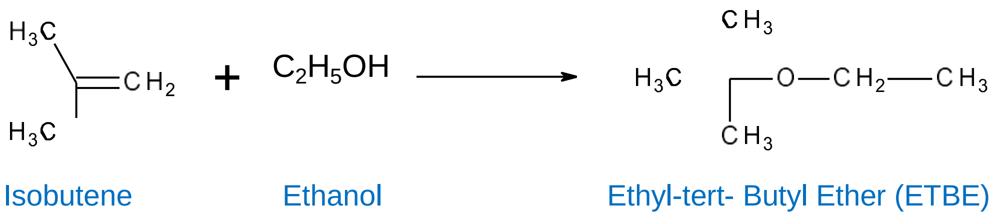
Table 10 Fact sheet 1st generation bioethanol production

Raw materials	Carbohydrate			
	- Sugar:	Sugar cane, sugar beet		
	- Starch:	Wheat, barley, rye, triticale, corn		
Products	Ethanol	→ Admixture to OK (Super 95, E10, E85)		
		→ Refining to ETBE		
By-products	Schlempe	→ after drying: feed		
		→ Substrate in biogas plants		
Yields		area-related	energy-related	mass-related
	Wheat	62 GJ/ha	56,0 % (Corn)	30,4 %
	Corn	83 GJ/ha	60,3 % (Corn)	31,6 %
	Sugar beet	162 GJ/ha	54,3 % (Turnip)	8,7 %
	Sugar cane	135 GJ/ha	36,9 % (Plant)	7,0 %
GHG emissions g CO2 eq/MJ		Standard (REDII)	typical (REDII)	certified (BLE)
	Wheat	31 - 72	31 - 60	11,4
	Corn	30 - 68	30 - 56	10,1
	Sugar beet	23 - 50	20 - 39	21,5
	Sugar cane	29	28	10,2
				On average (G) 11,0

Ethanol is miscible with gasoline in any ratio and can therefore be blended with conventional gasoline as a drop-in component. The high knock resistance, expressed by research octane numbers (RON) of 108-109 [53], [54] can, with appropriate optimization of the engines, lead to an increase in engine efficiency and thus to a reduction in specific, energy-related fuel consumption [54]. At the same time, emissions of hydrocarbons, carbon monoxide and nitrogen oxides are reduced. Due to the high oxygen content of 34.8 Ma.-%, ethanol has a calorific value of only 26.8 MJ/kg and thus a volume-related storage density that is about 35% lower than gasoline. The low vapor pressure leads to poor cold-start behavior at high ethanol contents in the fuel. In addition, ethanol has good solubility for various materials. This results in limitations when blending with conventional gasoline. If this is not the case, the engines and fuel systems must be adapted (see also section 4.2.1).

Only anhydrous ethanol is suitable for use as a fuel additive, since in mixtures of gasoline and hydrous ethanol the water precipitates and accumulates in the fuel system (corrosion). During dehydration, a so-called stillage is produced, which contains by-products such as fibers, proteins, and fats. These can be used as protein-rich animal feed or supplied for energy recovery (biogas, heat) [55]. Ethanol - like methanol - can be converted into the corresponding tert-butyl ether with the aid of isobutene (equation (3)), which can be used as a knock improver for conventional fuels.

(3)



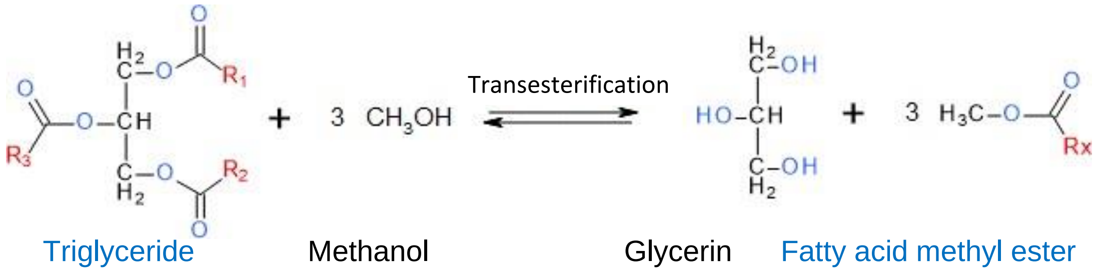
3.2.2. Biodiesel (FAME, UCOME)

From a chemical point of view, vegetable oils and animal fats are so-called triglycerides. In purely formal terms, these are esters of long-chain acids (fatty acids) with the trivalent alcohol glycerol. These oils are basically suitable for diesel engine combustion. However, the high viscosity and poor ignition properties in particular lead to application problems in vehicle operation, especially in winter or during cold starting:

- reduced pumpability (-> increased wear of pumps and injection systems),
- poor atomization (-> ignition delay and noise development - "nailing")
- Soot formation, deposits, clogging,
- lubricating oil dilution (unburned fuel deposits on the cylinder wall and thus gets into the engine oil).

Transesterification with methanol according to equation (3) produces fatty acid methyl esters (FAME), which have application properties very similar to those of conventional fuels. The product has been launched on the market as biodiesel.

(4)



A simplified process diagram is shown in Figure 27. Table 10 summarizes important characteristics for the production of biodiesel.

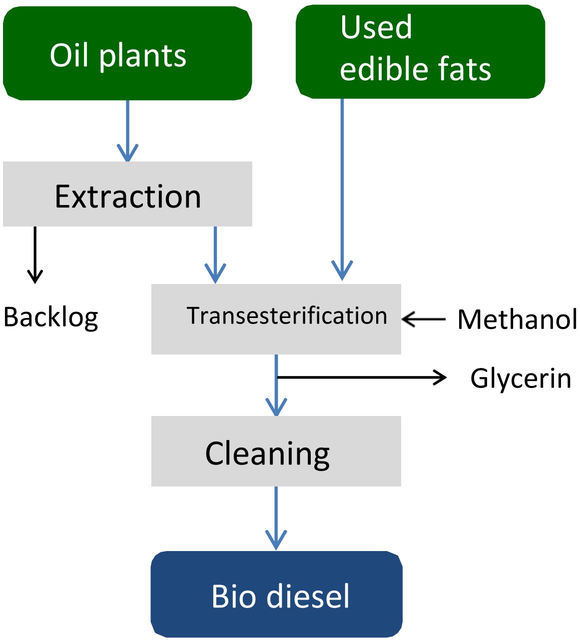


Figure 27 Process diagram for the production of biodiesel (FAME)

Table 11 Biodiesel production fact sheet

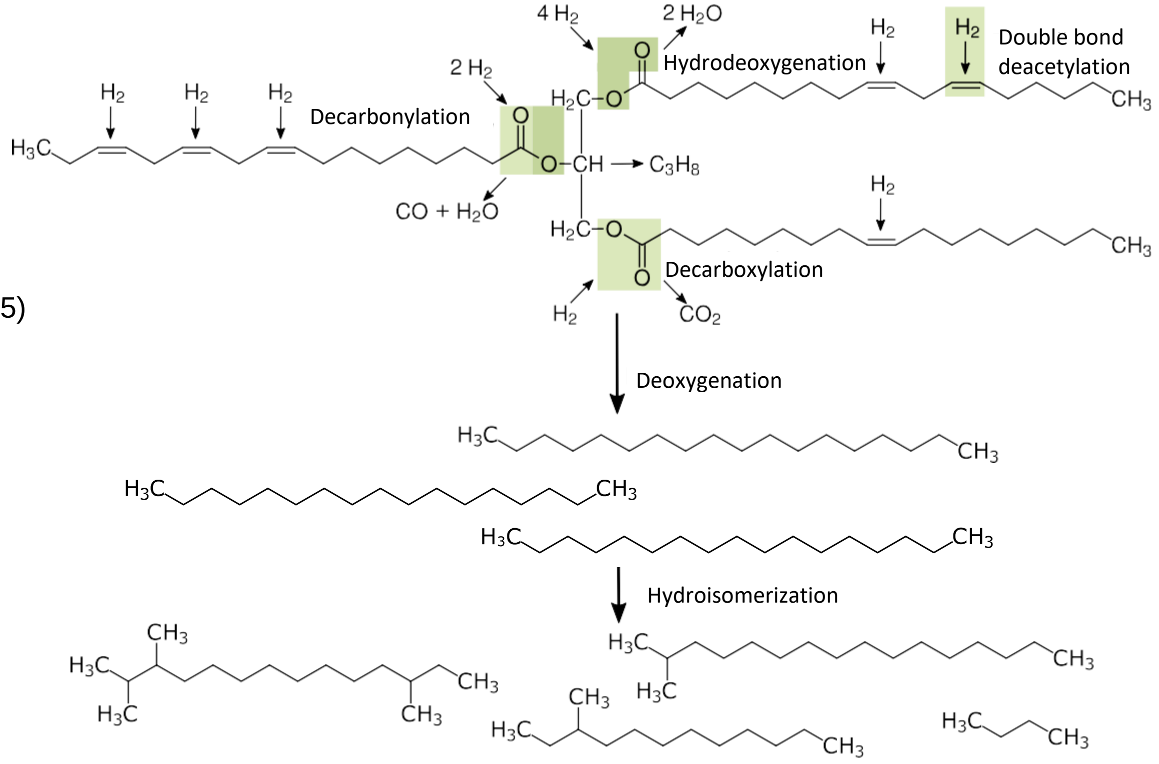
Raw materials	in principle all oil plants (e.g. rapeseed oil, palm oil), used edible fats, (animal fats)			
Products	Substitutes for diesel fuel and EL heating oil (specification DIN EN 14214), compared to conventional products: - slightly lower energy content, - higher water affinity (corrosion, storage stability) - chemically unsaturated (stability)			
By-products	Extraction residues (meal) as high-protein cattle feed Glycerin: as moisture retainer (cosmetics, tobacco), chemical raw material, energy carrier			
Yields		area-related	Energy related	Mass related
	RME	58 GJ/ha	63,3 % (Corn)	
	PME	145 GJ/ha	52,2 % (Fresh fruit)	
	UCOME		97,8 % (Used grease)	
GHG emissions g CO2 eq/MJ Raw materials		Standard (REDII)	typical (REDII)	certified (BLE)
	RME	50	46	32,4
	PME	52 - 76	46 - 64	23,3
	UCOME	15	11	6,9
				on average (D)
				18,4

Fatty acid methyl esters (FAME) are long-chain molecules with a similar size and structure to typical middle distillate components (e.g. n-hexadecane). Characteristic features are the ester groups as well as a varying number of double bonds (depending on the feedstock), which strongly determine the properties of the products.

Glycerol, which is a by-product (about 10.5 Ma.-% based on FAME), is used in a variety of applications (e.g. cosmetics industry, tobacco industry) due to its water-binding properties. It can also be used as a raw material in the chemical industry or as an energy source.

3.2.3. Hydrogenated vegetable oils (HVO)

The hydrogenation of vegetable oils represents an alternative to the transesterification of oils and fats. The reaction with hydrogen both saturates the double bonds of the fat molecules and removes the oxygen contained in the ester groupings in the form of water or carbon oxides (equation 5). The products obtained are a mixture of kerosenes in the boiling range of diesel fuel. The chain lengths (C number) of the products depend on the fatty acid profile of the oils used. The primarily formed unbranched n-alkanes usually have relatively high melting temperatures and thus poor low-temperature properties. They must therefore be subjected to isomerization in a second process step [56], [57]. In this process, cracking processes also occur as a side reaction, which shift the boiling point of the product and can be associated with yield losses. With increasing isomerization severity, the proportion of light fractions (kerosene, naphtha) increases [58]. The very light components are generally undesirable in this process because they are not suitable for use as gasoline.



(5)

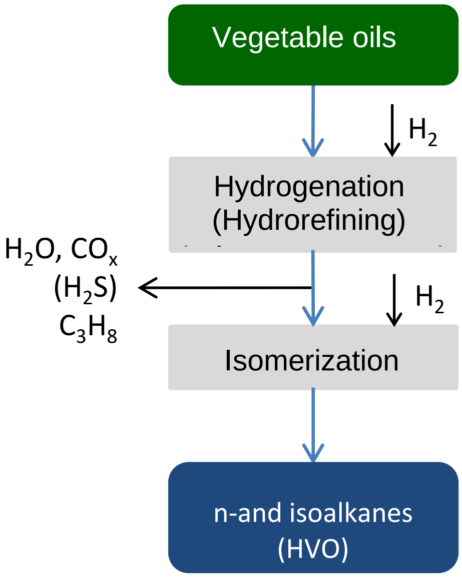


Figure 28 Process diagram production of hydrogenated vegetable oil (HVO)

HVO or HEFA is similar to the synthetic diesel, fuel oil and kerosene substitutes, which are also paraffinic and originate from the Fischer-Tropsch synthesis. The paraffinic products burn with less soot, have a high ignition propensity (cetane number) and, due to their lower density, a somewhat lower volumetric calorific value. The refrigeration properties can be adjusted by isomerization (see also section 4.2.2).

Table 12 Hydrogenated vegetable oil production fact sheet

Raw materials	all fats and oils, also with free fatty acids, currently mainly palm oil and waste oils			
Products	High-quality middle distillates for use as DK or EL heating oil as well as Jet A1 (paraffin-rich, high cetane number, sulfur- and free of aromatics; cold resistance can be adjusted as required)			
By-products	Propane	- provision of process energy, - biogenic liquefied gas		
Yields		Area related	Energy related	Mass related
	Rapsl-HVO	57 GJ/ha	61,8 % (Corn)	
	Palmöl-HVO	142 GJ/ha	51,1 % (Fresh fruit)	
	UCO-HVO		95,5 % (Used grease)	
	Hydrogenation	80 … 87 Ma. -% (Ref. to feed oil)		
GHG emissions g CO2 eq/MJ		Standard (REDII)	typical (REDII)	certified (BLE)
	Rapsl-HVO	50	46	
	Palmöl-HVO	48 - 73	44 - 62	
	UCO-HVO	16	12	
				on average (D) 19,5

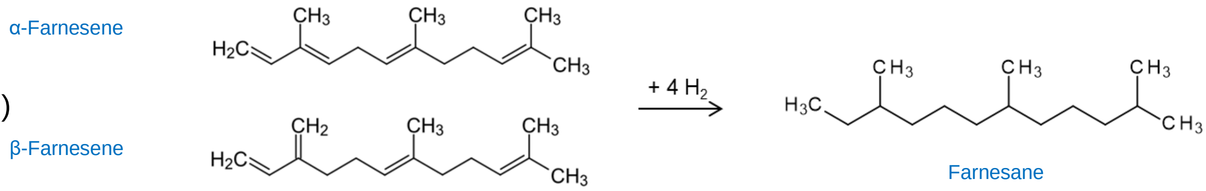
The hydrogen demand required for hydrogenation of the double bonds or hydrodeoxygenation to remove oxygen can be reduced by thermal treatment upstream of hydrogenation [59]. In this case, most of the oxygen is split off in the form of carbon oxides. At the same time, the process leads to a broader boiling distribution of the products.

3.2.4. Farnesene

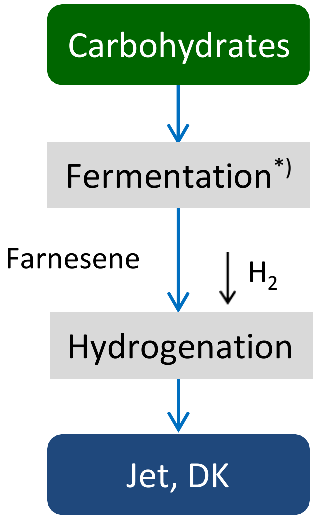
In addition to the production of alcohols, fermentations also offer the possibility of directly producing very specific oxygen-free hydrocarbons by biological means. One example of this is Farnese. These are unsaturated, regularly branched hydrocarbons with 15 carbon atoms that belong to the group of terpenoids. They can be technically produced by yeasts from carbohydrates to which genes of the annual mug wort (artemisia annua) for fern synthesis have been transferred by gene transfer [60].

After saturation of the double bonds by hydrogenation, the substance is called farnesane. Due to the degree of branching, it has a very low cloud point of -78 °C [61] and a boiling point around 250 °C and is therefore very suitable as jet fuel. It can also be considered for use as diesel fuel or heating oil.

(6)



The general production scheme is shown in Figure 29. Table 13 contains a fact sheet.



*) with special yeasts

Figure 29 Process diagram production of farnesol

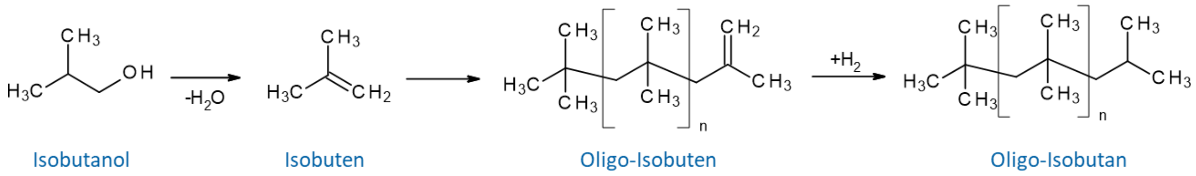
Table 13 Fact sheet production of Farnese

Raw materials	Carbohydrate-containing biomass, e.g. sugar cane			
Products	multi-branched C15 alkanes - very good cold resistance (Jet) - high cetane number (DK)			
By-products	None			
Yields		Area related	Energy related	Mass related
	Sugar cane	113 GJ/ha	30,8 % (Plants)	
GHG emissions g CO2 eq/MJ		Standard (REDII)	typical (REDII)	Literature
	Sugar cane	k. A.	k. A	45 [62]

3.2.5. Jet fuel from alcohols

Alcohols produced by fermentation can also be used to produce hydrocarbons for jet fuel. In the alcohol-to-jet process (see Fig. 30), the alcohols are first dehydrated to alkenes.

(7)



These can then be oligomerized. If a branched alcohol, such as isobutanol, is used, the oligomerisates are also highly branched, regardless of the oligomerization process. However, unbranched alcohols can also be used; oligomerization on acidic zeolites also produces highly branched products. In the subsequent distillative separation, the oligomers in the desired boiling range are separated as a product stream and the remainder is recycled to increase the yield. The product is still unsaturated and is finally hydrogenated to saturated hydrocarbons.

These are very highly branched, and the boiling point can be adjusted via the distillation mode. The product is thus very well suited as a substitute for jet fuel, but use as diesel fuel or heating oil would also be possible.

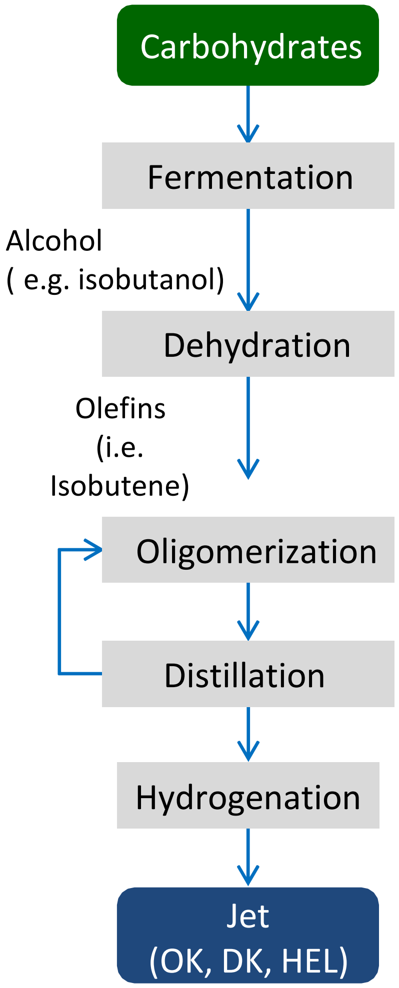


Figure 30 Alcohol-to-Jet process diagram (AtJ)

Table 14 AtJ-Jet production fact sheet

Raw materials	Biomass containing carbohydrates, e.g. sugar cane or corn			
Products	Biomass containing carbohydrates, e.g. sugar cane or corn			
By-products	Stillage	- after drying: feed - Substrate in biogas plants,		
Yields		Area related	Energy related	Mass related
	Sugar cane	120 GJ/ha	32,8 % (Plant)	
GHG emissions g CO2 eq/MJ		Standard (REDII)	typical (REDII)	Literature
	Sugar cane	k. A.	k. A.	22 [62]
	Wheat straw	k. A.	k. A.	30 [63]

3.3. Advanced biofuels (excluding BtL)

Advanced biofuels include all fuels produced from residual materials (see RED II, Annex IX A). They do not compete with food and feed production and are counted as 2nd generation fuels (see Table 4 on p. 23).

Such residues (e.g., wood waste, straw) consist mainly of lignocellulose, from which 2nd generation ethanol (2G ethanol), biomethane, or bio-pyrolysis oils can be produced [64]. Furthermore, biomass can also be converted into a synthesis gas by means of gasification, from which a wide variety of synthetic fuels can be produced via different reaction pathways. These biomass-to-liquid (BtL) processes are described in section 3.4.

3.3.1. 2G-Ethanol

Lignocellulose consists of three main components, of which cellulose and hemi-cellulose are fermentable carbohydrates. Another important component is lignin, which acts as a binder for cellulose/hemi-cellulose and gives the wood or straw its strength. Lignin is not fermentable. In order to make the cellulose or hemi-cellulose accessible to fermentation, the lignocellulose must first be digested, which makes 2G ethanol recovery significantly more complex than the classic alcoholic fermentation of substrates containing starch or sugar (Figure 31).

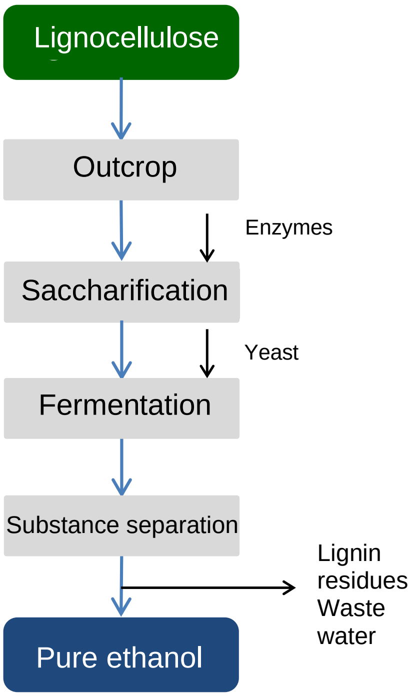


Figure 31 Process diagram production of 2nd generation bioethanol

There are several chemical or physical-chemical process options for digestion. These include acid digestion, basic digestion, digestion with water (under pressure), each of which can also be carried out as a "steam explosion" process, in which the pressurized suspension is suddenly expanded [65], [66]. The digested cellulose is then broken down enzymatically (cellulases) into the individual sugar monomers. Cellulose is converted into glucose, whereas hemicellulose is converted into a mixture of xylose, mannose, arabinose, and galactose. Unlike the other sugars mentioned, xylose and arabinose are pentoses (C5 sugars), which are not metabolized by standard yeasts for 1G ethanol production (saccharomyces cerevisiae). Therefore, the use of specialized yeasts that can utilize both C5 and C6 sugars is required [66], [67]. Finally, the ethanol is obtained by distillation. The lignin and other residues can be thermally recycled.

Of course, 2G ethanol does not differ materially from conventional bioethanol. Thanks to the different raw material base, however, it is not subject to the restrictions on its eligibility as a renewable energy source for meeting quotas under REDII or BImSchG. Only fuel standardization imposes blending limits (e.g., E5, E10, E85).

Table 15 2G ethanol production fact sheet

Raw materials	Lignocellulose (straw, waste wood)			
Products	Ethanol	Blending to OK Refining to ETBE		
By-products	Lignin energy use (process energy, sale)			
Yields		Area related	Energy related	Mass related*)
	Waste-wood		41,1 %	26,2 %
	straw	50 GJ/ha	35,7 %	22,4 %
GHG emissions g CO2 eq/MJ		Standard (REDII)	typical (REDII)	models
	Cultured wood	k. A.	k. A.	20
	Waste wood	k. A.	k. A.	9
	Straw	16	13	8

*) based on dry matter

3.3.2. Bio oils

With the aid of thermal-chemical processes (such as pyrolysis, hydrothermal liquefaction, chemical pulping), it is comparatively easy to obtain liquid or oily products from biomasses. In principle, these are suitable for further processing into fuels, but this is extremely costly due to the mostly very unfavorable properties of the primary products. Bio-oils, such as pyrolysis oils from wood waste or sewage sludge, hydrothermally liquefied algae biomass or also tall oils (by-product of pulp production) are complex mixtures with high contents of heteroatoms (nitrogen up to 7 Ma.-%, oxygen up to 30 Ma.-%). They are usually highly unsaturated, polar and also often viscous liquids.

For the necessary upgrading to adjust the required application properties (boiling point, heteroatom content, viscosity, calorific value, low-temperature properties, ignitability, anti-knock properties), the known refinery processes, in particular hydrotreating/hydrocracking, are suitable. However, the use of such bio-oils can lead to rapid catalyst poisoning and is associated with high hydrogen consumption. Moreover, the removal of heteroatoms leads to a partial cleavage of the molecules associated with a lowering of the boiling point. Hydrogenated bio-oils have a broad boiling distribution throughout the range of target products (naphtha, kerosene, diesel).

Against this background, a local application of such oils as non-standard fuel for heat supply appears to be a better option compared to the extraction of high-value sales products.

3.4. Synthetic Fuels

3.4.1. Overview

Among the various processes for producing advanced fuels, those using synthesis gas occupy a special position. Synthesis gas is a mixture of hydrogen and carbon monoxide. It can be produced from both fossil sources and renewable sources and can be used as a feedstock for a variety of possible products (see Figure 32). When biomass is used as a source, the term "biomass-to-X" (BtX) process is used. When electricity, preferably renewable, is used with carbon dioxide as the carbon source, the processes are referred to as "Power-to-X"(PtX) processes.

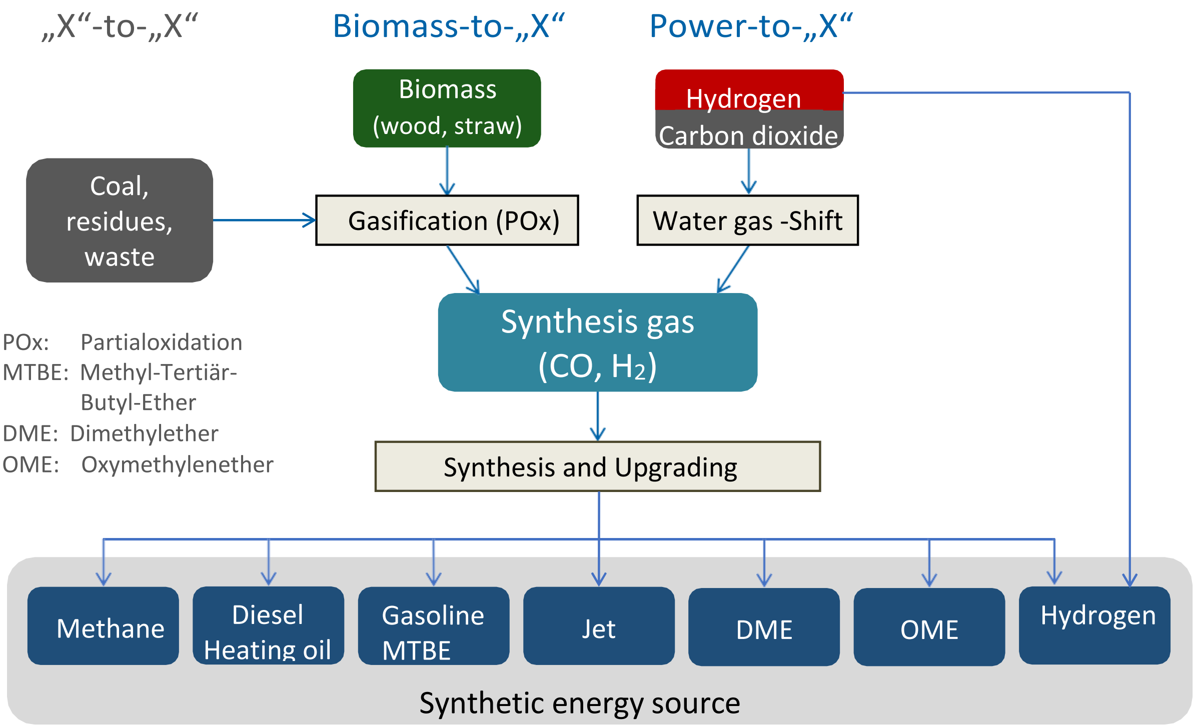


Figure 32 Synthetic fuels - Overview of raw materials and products

The synthesis gas generated can be converted into the desired target product via various syntheses. The raw material and product properties are decoupled via the synthesis gas interface. If liquids are produced, in the case of BtX and PtX the "X" is referred to as "liquid", i.e. abbreviated as BtL or PtL. When gases are produced, correspondingly as "gas", which can be abbreviated to BtG or PtG.

The product properties can be adjusted in a targeted manner via the choice of the substance to be produced or, if necessary, also via the parameters of the synthesis, in some cases in a tailor-made manner. The required synthesis technologies (e.g. methanol synthesis or Fischer-Tropsch synthesis for the production of hydrocarbons) are largely known and are already used on a large industrial scale. However, currently coal or gas is mostly used as feedstock. Each synthesis requires a specific ratio between H2 and CO, which can be adjusted via the water gas shift reaction (equation 8).

(8) Water gas shift reaction: $CO + H_2O \leftrightarrows CO_2 + H_2$

The molar ratio for most syntheses is about 2:1 (H_2:CO). Biomass gasification, on the other hand, yields ratios closer to 1:1. Via the water gas shift reaction, water has to be converted into H2 to set the necessary ratio. In the process, part of the CO is consumed. In PtX processes, pure hydrogen is initially produced in the electrolysis. To provide the required CO, CO2 is reacted with a portion of the H2 via the reverse water gas shift reaction[8]. Alternatively, the direct conversion of CO2 with H2 is also conceivable. However, CO2-based syntheses are current part of research and technically not yet established.

A major advantage of BtX technologies is that virtually any biomass can be processed, including lignocellulosics such as wood or straw. Raw materials can be used that do not compete with food or feed crops. Therefore, depending on the exact biomass used, BtX products are also considered advanced biofuels.

In the long term, there is an even greater potential for renewable electricity and thus also for PtX products (e-fuels). In addition to their use as power or fuel, these can also be used to chemically store fluctuating wind or solar power. If required, they can be converted back into electricity. Furthermore, they make it easier to import renewable electricity-based energies. Transporting electricity over long distances is difficult and involves high losses. Liquid PtX products, on the other hand, are comparatively easy to transport worldwide.

3.4.2. Synthesis gas production

Biomass gasification

Gasification processes in which the biomass is incompletely oxidized are used to generate synthesis gas from biomass. Many possible process variants (including partial oxidation with O2 or allothermal gasification with H2O; high or low pressure; fluidized bed or entrained flow) are available for this purpose [68]. Before the actual gasification, a pretreatment of the biomass to a more homogeneous, easily dosed intermediate product is necessary (e.g. torrefaction [22], pyrolysis [69]). This reduces the water content. At the same time, the energy density of the feedstock increases considerably. In the case of decentralized pretreatment, the transport costs to the central gasification plant can thus be reduced. Against the background that gasification plants operate more economically the larger they are, the transport costs are an important parameter for the optimum size of the biomass catchment area of a BtX plant. The main products of gasification are carbon monoxide and hydrogen, the synthesis gas. By-products are carbon dioxide, water, and organic compounds ranging from methane to tar. Other by-products, such as ammonia and hydrogen sulfide, come from the nitrogen and sulfur content of the biomass. Tar formation is largely determined by process control and is particularly relevant in fluidized bed gasification, which operates at lower temperatures. The synthesis gas is purified from these by-products and brought to an H2 to CO ratio required for the subsequent synthesis by means of a water gas shift reaction (see Fig. 33).

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[8] the reverse reaction of the water gas shift reaction

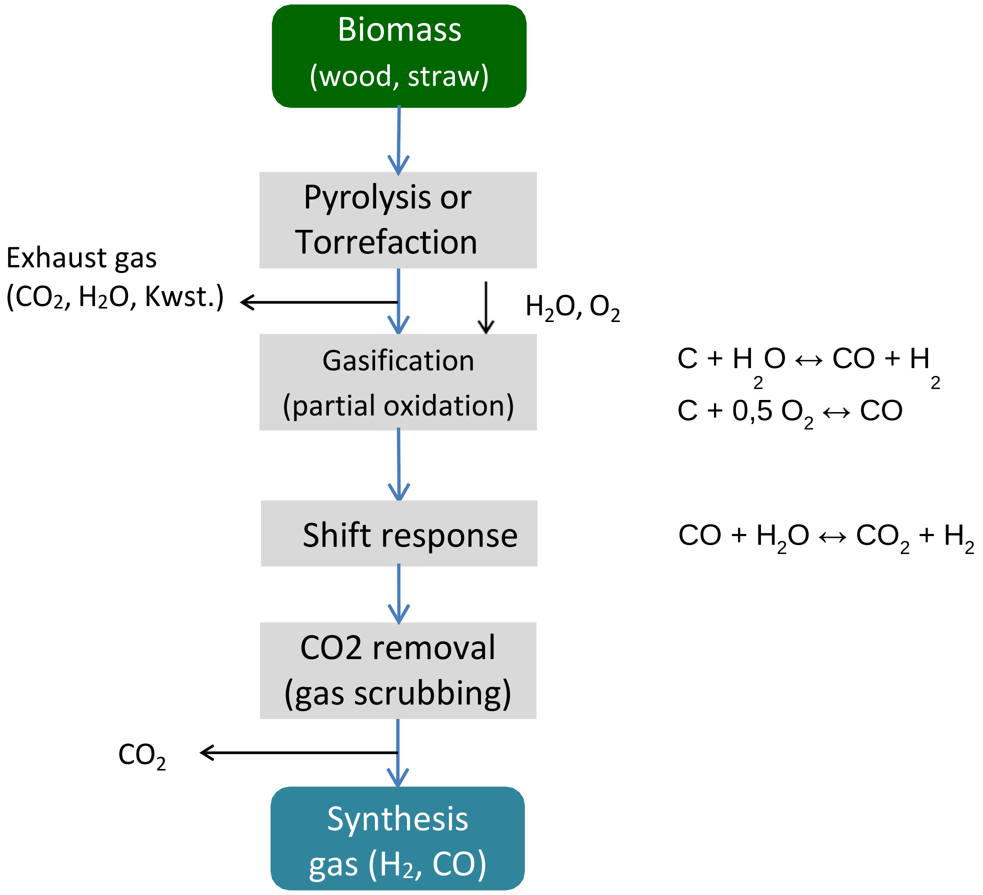


Figure 33 Process diagram biomass gasification

Synthesis gas itself is difficult to transport and is usually converted into the actual product, or even an intermediate product, at the site of its generation with a subsequent synthesis (see chapter 3.4.3)

Table 16 contains a fact sheet on biomass gasification.

Table 16 PROFILE Synthesis gas production (biomass gasification)

Raw materials	Lignocellulose (straw, waste wood), lignin, energy crops			
Products	Intermediate synthesis gas (H_2/CO mixture) → Methanol → OK, DME, OME → Fischer-Tropsch products			
By products	no value products combustible gases produced: Coverage of own energy demand			
Yields		by area	energy-related	Mass related *)
	Waste wood		67 %	49,8 %
GHG emissions g CO_2 eq/MJ		Standard (REDII)	Typical (REDII)	Modeled
	Cultivated Wood	N. A.	N. A.	2
	Waste wood	N. A.	N. A.	8
	Straw	N. A.	N. A.	3

*) Based on dry matter

Electricity-based synthesis gas

For the material use of electrical energy, the energy is stored in the resulting hydrogen by means of electrolysis of water. Oxygen is produced as a by-product:

(9) Water electrolysis: $2\ H_2O \rightarrow 2\ H_2 + O_2$

For electricity-based synthesis gas, a carbon source is also required. CO2 is usually used, which comes from a point source or can be captured from the air. The syngas is obtained via the reverse water-gas shift reaction (equation 8), in which part of the hydrogen produced by electrolysis is converted with CO2 to CO (see Fig. 34).

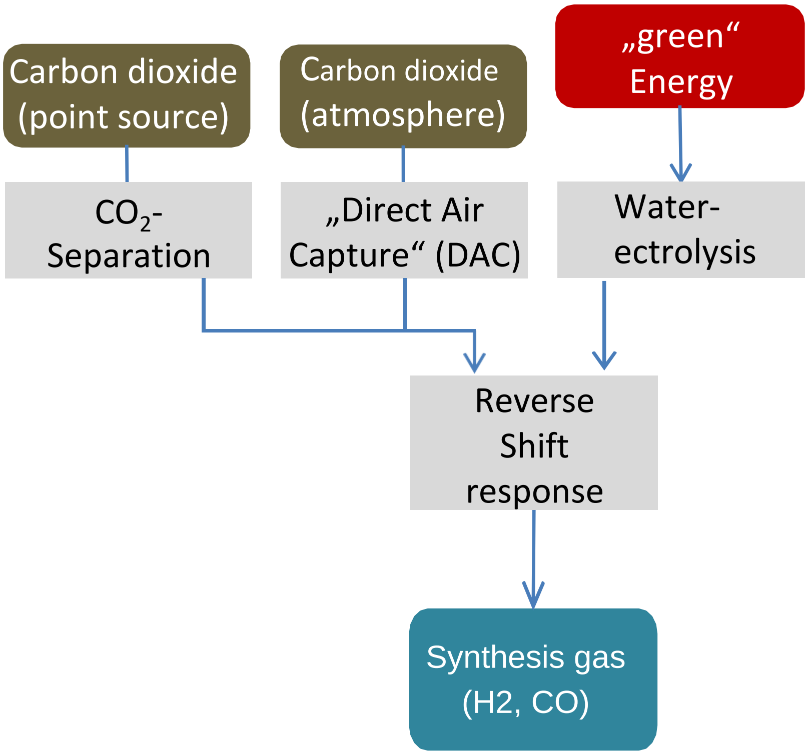


Figure 34 Process schematic synthesis gas from CO2 and e-electricity

Hydrogen production - electrolysis

The use of electrical energy for the electrolytic production of hydrogen takes place in so-called electrolyzes. An electric current is applied therein, which is conducted through ionic conduction in the electrolyte with which the electrolyzer is filled. Electrons are released and absorbed at the cathode and anode, respectively, and lead to the production of hydrogen and oxygen, respectively, through electrochemical reactions. An ion-permeable but gas-tight separating layer (e.g., a membrane) prevents the product gases from mixing.

Electrolysis processes are divided into three important genera:

- *Alkali electrolysis:* Low-temperature process (50 - 80 °C) in which a potassium hydroxide solution is used as the electrolyte. The membrane allows the exchange of OH- ions. The reactions at the cathode and anode are:

  (10) Cathode: $4\ H_2O + 4\ e^- \rightarrow 2\ H_2 + 4\ OH^-$

  (11) Anode: $4\ OH^- \rightarrow 2\ H_2O + 4\ e^- + O_2$

Alkali electrolysis is state of the art and is already being used on a large scale. It can be operated at atmospheric pressure, or at pressures up to 30 bar, and can be adapted relatively flexibly to a fluctuating power supply. However, alkali electrolysis requires a certain start-up time and a minimum load of approx. 10 % of its maximum capacity.

- *Proton exchange membrane (PEM) electrolysis:* Low temperature process like alkali electrolysis. The anode and cathode are located on two different sides of a polymer membrane that allows H+ ions (protons) to pass through. Water is usually added as the electrolyte on the anode side, which is partially split by the applied current to form H+- ions and oxygen. Due to the presence of H+ ions, the medium becomes acidic. The reactions at the cathode and anode are:

  (12) Cathode: $4\ H^+ + 4\ e^- \rightarrow 2\ H_2$

  (13) Anode: $2\ H_2O \rightarrow 4\ H^+ + 4\ e^- + O_2$

  One of the advantages of PEM electrolyzers over alkaline electrolyzers is the ability to start up spontaneously, which is somewhat of an advantage when renewable power sources are often intermittent. It can even be run in overload mode for short periods. Operating pressures of up to 85 bar are possible [70]. Compared to alkali electrolysis, the stack lifetime is somewhat lower, as well as the capital costs somewhat higher.

- *Solid oxide electrolysis:* High-temperature process (approx. 850 °C) has a higher efficiency than the low-temperature processes because electrolysis is thermodynamically favored at higher temperatures. In addition, some of the heat to be applied can also come from process waste heat, for example from syntheses. The solid oxides have a conductivity for oxide ions. The reactions at the cathode and anode are*:*

  (14) Cathode: $2\ H_2O + 4\ e^- \rightarrow 2\ H_2 + 2\ O^{2-}$

  (15) Anode: $2\ O^{2-} \rightarrow O_2 + 4\ e^-$

  A disadvantage is that they are less suitable for rapid load changes than the low-temperature processes. Currently, the capital costs for these electrolysers are higher than those of low-temperature processes [8].

  Co-electrolysis can also be operated in these electrolysers by adding carbon dioxide in addition to water [71]. The following reaction then takes place at the cathode in addition to those mentioned above:

  (16) Cathode (Co-Electrolysis) $2\ CO_2 + 4\ e^- \rightarrow 2\ CO + 2\ O^{2-}$

  By means of co-electrolysis, synthesis gas can be directly produced electrolytically.

  Table 17 lists some characteristic values for the various types of electrolyzer. In solid oxide electrolysis, electrical efficiencies >100 % are possible by utilizing thermal energy.

Table 17 Overview of parameters of different electrolysis processes [8], [72], [73]

	Alkalish Elektrolysis		PEM-Elektrolysis		Solid oxide electrolysis	
	Today	2050	Today	2050	Today	2050
Operating temperature (°C)	to 100		to 100		150 to 1.000	
Pressure (bar)	1 – 30		1 – 85		5 – 50	
Stack power (kW)	to 6.000		to 225		to 150	
Operating load ()	20 – 100 %		10 – 166 %		30 – 100 %	
Lifetime (years)	8 – 15	25	6 – 10	25	3 – 10	(25)
Investment costs (€/kWh)	800	350	2000	250	2000	250
Energy demand (kWh/m^3 i.N.)	5 – 7	4	4 – 7	4	3 – 3,7	3
electr. efficiency (Hs)	65 %	80 %	65 %	80 %	95 %	119 %

Carbon dioxide production

Carbon dioxide, which acts as a carbon source for the electricity-based synthesis processes, can either be taken from a point source in which it is present in concentrated form or captured from the air (DAC - direct air capture) (cf. chapter 2.3).

Capture from air is very costly due to the extremely low CO2 concentration (410 ppm). Conventional physical scrubbing is unsuitable for this purpose, and extraordinarily large volumes of air have to be moved and treated (more than 1.3 million m^3 of air per ton of CO2). This entails correspondingly large plant technology and high energy expenditures (fans, regeneration of filters).

Currently, different technologies for chemisorption of carbon dioxide by both absorption and adsorption processes are being considered [8], [46], [74], focusing on the development of suitable sorbents and their regeneration. Three basic process variants are described:

- Electrodialysis in which the CO2 in the absorbing alkaline liquid (e.g. NaOH) is expelled by adding sulfuric acid. Recovery of the sulfuric acid and base is accomplished by an electrochemical membrane process.
- Calcination, in which the absorbed CO2 is precipitated as calcium carbonate (CaCO3). The calcium carbonate decomposes at high temperatures (calcination) to calcium oxide and pure CO2.
- Desorption processes in which the CO2 adsorbs on amine compounds (chemisorption) and can be selectively desorbed again by adding a small amount of heat in a vacuum.

The market leader is the Swiss company Climeworks, which already offers collectors with a capacity of 6 kg CO2/h (equivalent to about 50 t/a) commercially. The plants operate with a solid adsorbent based on amine-modified cellulose fibers according to the principle of temperature swing adsorption [74], [75]. The comparatively low temperature level (regeneration at 100 °C) allows the use of low-temperature heat in CO2 recovery and thus promises cost advantages over other process variants that require temperatures of more than 850 °C for regeneration [76]. The modules can be interconnected to form larger plants. For example, the company has been operating a demonstration plant with 18 modules and an annual capacity of 900 t CO2 since 2017 [75], [77]. Currently, a modular plant is under construction in Iceland to capture 4,000 annual tons of carbon dioxide from the atmosphere is being planned as the largest of its kind to date [78]. About 85 such plants would be needed to produce 100,000 t/a of synthetic fuels.

Table 18 shows the key data for various processes taken from the literature for capturing CO2 from air.

Table 18 CO2 capture fact sheet - Direct Air Capture (DAC)

Desorptions-temperature (°C)	**Procedure principle** *)	**Energy demand (MWh/t CO_2)**				**Costs (€/t CO_2)**		**Source**
		total	thermal	electric	Fan energy	today	With learning curve	
-	-	2,5				911	273	[79]
130	D	1,7	0,7	1	0,83	688 - 1114		[80]
900	C	2,8	2	0,8	0,56			[81]
-	C	-			0,09	467		[82]
900	C	1,8	1,4	0,4	0,06			[83]
900	C	2,1	1,7	0,4	0,17		100 - 144	[84]
-	E	2,3 - 3,4		2,3 - 3,4				[8]
-	E	1,9		1,9				[8]
850	C	2,8						[8]
95	D	1,7 - 2,3	1,5 - 2,0	0,2 - 0,3	0,2 - 0,3			[8]
-	E	2,3		2,3		477 - 493	312 - 321	[8]

*)C – calcination, D - desorption, E - electrodialysis

The extraction of CO2 from point sources is associated with significantly less effort, since the CO2 is present in a more concentrated form. The basic process is comparable to CO2 capture from air. However, due to the much lower gas flows, other contacting methods can be used. Table 19 lists the costs for CO2 capture from point sources according to literature data.

Table 19 Fact sheet CO2 capture - point sources (industrial waste gases)

Origin	**Costs (€/t CO_2)**		**Source**
	today	2050	
Coal-fired power plant	26,6 - 33,9	< 30	[85]
Gas-fired power plant	57,7 -111,8		
Cement industry*)	43		[13]
Blast furnace gas/refineries*)	61		
Steel industry*)	82		
Ammonia synthesis*)	112		

*) inkl. Compression

The cost of providing the carbon dioxide is a major price component for the synthetic energy sources produced from it (see Figure 35). In this context, even under favorable conditions (low electricity costs), DAC burdens the price considerably more than the use of point sources (factor 5-10). Assuming a CO2 price of 300 €/t CO2, the use of DAC results in costs of 70 ct/l product for the stoichiometrically necessary CO2 quantity alone.

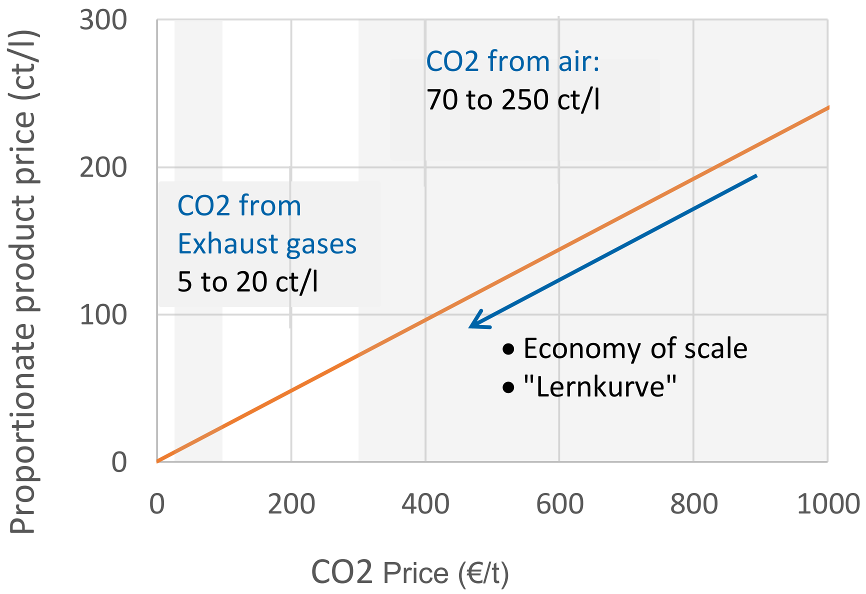


Figure 35 Influence of CO2 price on fuel costs (pro rata) for PtL products from Fischer-Tropsch synthesis.

The exact ratio of H2 to CO in the syngas is adjusted via the reverse water gas shift reaction, in which the necessary proportion of hydrogen is converted with CO2. Table 20 shows a profile for electricity-based synthesis gas production.

Table 20 Profile of synthesis gas generation (e-electricity and CO_2)

Raw materials	"Green" electricity and CO2 from point sources and atmosphere, respectively.		
Products	Intermediate synthesis gas (H2/COx mixture) -> Methanol ->OK, DME, OME ->Fischer-Tropsch products		
By-products	no valuable products combustible gases produced: Coverage of own energy demand		
Yields		energy-related	mass-related
	Hydrogen:		0,019 kg/kWh
	Syngas	63 %	
	- without DAC	62 %	
	- with DAC	50 %	
GHG emissions		Standard (according to 37. BImSchV)	models
g CO2 eq/MJ	Hydrogen:	9	11
	Syngas		
	- without DAC		
	- with DAC	k. A.	11
		k. A.	13

3.4.3. Fuel Syntheses

Fischer-Tropsch synthesis

Fischer-Tropsch synthesis is well established on an industrial scale and, along with ammonia and methanol synthesis, is one of the most important uses of synthesis gas [68]. A mixture of predominantly unbranched hydrocarbons with a broad distribution of C-numbers is produced. A generalized reaction equation is as follows:

(17) Fischer-Tropsch-Synthesis: $n\,CO + n\,H_2 \rightarrow n\,\text{-}CH_2\text{-} + n\,H_2O$

The term -CH2- stands for individual segments of the hydrocarbon chains. The products consist mainly of kerosenes and olefins. Oxygenates (alcohols, ethers) and aromatics are also formed via side reactions. The chain length distribution can be approximately described by an Anderson-Schulz-Flory distribution. The mass fraction wn of components with a chain length of n carbon atoms is given by the following equation:

$$w_n = n(1-\alpha)^2\alpha^{n-1} \quad (18)$$

The parameter α is called chain growth probability and describes the probability for the incorporation of a further -CH2- unit before the reaction stops by desorption of the chain from the catalyst surface. It depends on the catalyst used and can be influenced by the reaction conditions (temperature, CO/H2 ratio). The resulting distribution of the chain lengths is shown in Figure 36, summarized in substance groups.

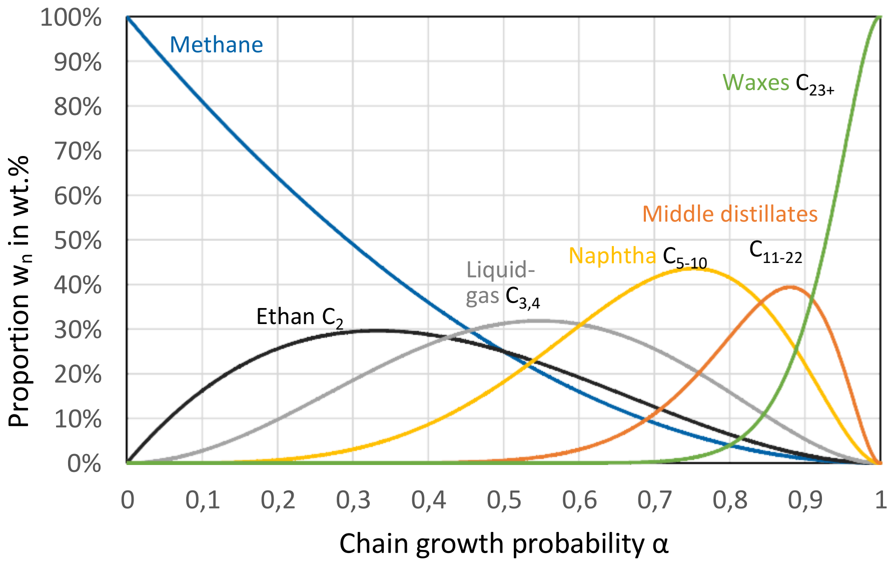


Figure 36 Product spectrum as a function of chain growth probability, according to Anderson-Schulz-Flory distribution [86]

Iron, cobalt or ruthenium are suitable catalysts. The reaction is carried out at elevated temperatures of 200 to 350 °C and pressures of approx. 30 bar. A distinction is made between low-temperature and high-temperature Fischer-Tropsch synthesis (LTFT9 and HTFT10, respectively). In LTFT, which is usually carried out with cobalt catalysts, rather long chains (large α) and few unsaturated compounds are formed. In HTFT - where iron catalysts are more commonly used - shorter chain products (smaller α) and more unsaturated compounds (olefins and aromatics) are formed. The reaction is generally highly exothermic and must be actively cooled; tubular reactors or slurry reactors are used as reactors, for example. Fluidized bed reactors are also used for HTFT.

The resulting product mixture, so-called Fischer-Tropsch crude[11] or Syncrude, usually consists of many different fractions. If middle distillates are to be produced specifically, it is favorable to work at a high chain growth probability (>0.9) [87]. At α ≈ 0.9, a maximum for kerosene/diesel can be expected in the primary products. Parallel long-chain waxes can be converted into additional middle distillates by downstream hydrocracking (see Figure 37). In this process, olefins and oxygenates are also hydrogenated to kerosenes. In addition, isomerization takes place, which significantly improves the low-temperature properties. The n-paraffins produced in the Fischer-Tropsch synthesis have comparatively high melting points. Distillate fractions can also be isomerized selectively, in which case cracking processes take place as a side reaction. The formation of naphtha is suppressed at high chain growth probabilities. This is advantageous because the primary FT gasoline is characterized by poor knock properties (octane number below 40 [88]) and therefore requires relatively complex upgrading in order to be usable as gasoline [89].

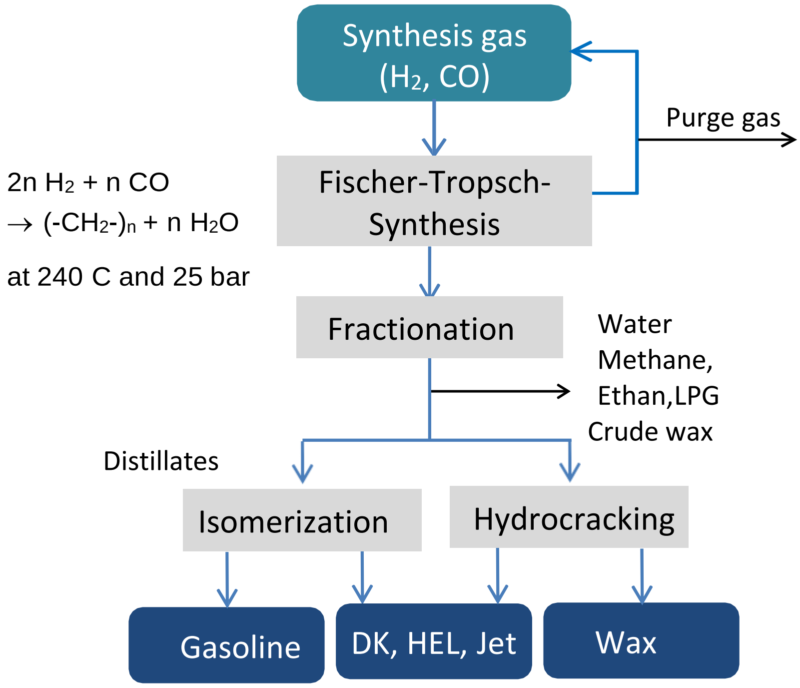


Figure 37 Process diagram Fischer-Tropsch synthesis

The middle distillate product resulting from the Fischer-Tropsch synthesis is a paraffinic diesel fuel or jet fuel whose technical properties hardly differ from hydrogenated vegetable oil(p. 42) due to its very similar chemical composition. Table 21 contains a fact sheet on the Fischer-Tropsch synthesis.

---

[9] LTFT – *low temperature Fischer Tropsch*
[10] HTHT – *high temperature Fischer Tropsch*
[11] Based on the English term crude oil for raw (earth) oil

Table 21 Fact sheet Fischer-Tropsch synthesis

Raw materials	Synthesis gas			
Products	n-paraffin mixture with broad chain length distribution → DK, HEL, Jet → (OK)			
By-products	Heating gas, LPG energy use (process energy, sale)			
Yields	per pass: max. 50 % (> 95 % with closed-loop control) energy efficiency: 69 % (without waste heat recovery)			
GHG emissions		Standard (REDII)	typical (REDII)	model
g CO2 eq/MJ Raw materials	Cultured wood	14	14	4
	Waste wood	17	17	12
	Straw	k. A.	k. A.	5
	e-electricity	k. A.	k. A.	16
	e-Electricity +DAC	k. A.	k. A.	18

Methanol synthesis

Another important product currently produced on a large scale from synthesis gas is methanol, the simplest alcohol.

(19) Methanol synthesis: $CO + 2\ H_2 \rightarrow CH_3OH$

The synthesis is technically carried out at pressures of 50 to 150 bar and temperatures of 230 to 270 °C [90] (Figure 38).

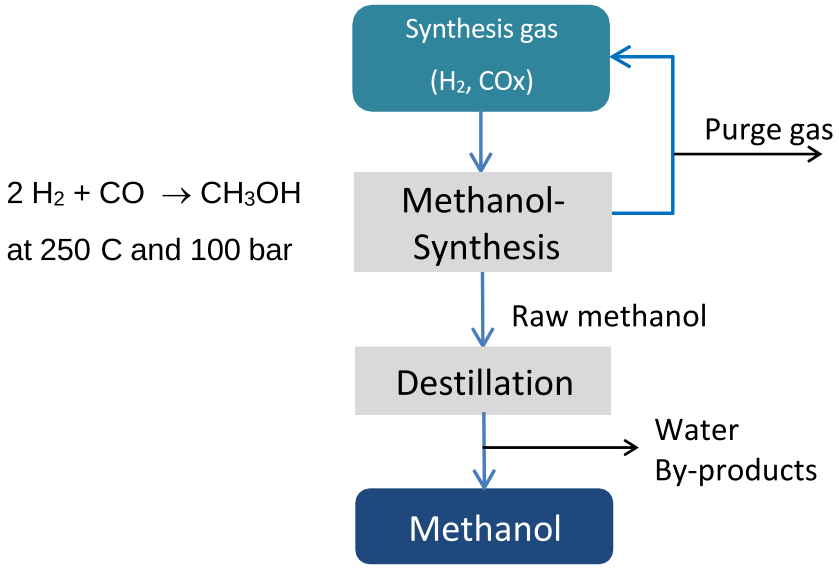


Figure 38 Process diagram methanol synthesis

Copper-zinc oxide catalysts are used as catalysts. From a thermodynamic point of view and due to the temperature-sensitive catalyst, the exothermic reaction requires very good heat dissipation or cooling of the system. Reactor types to be considered are shell-and-tube reactors, in which the heat is removed by evaporation of a water stream, or horde reactors with intercooling by cold gas quench streams.

The reaction is equilibrium limited; high pressures and low temperatures shift the equilibrium of the reaction toward methanol. This limitation of the equilibrium means that high conversion cannot be achieved in the reactor. The unreacted part of the synthesis gas is therefore recycled (see Figure 38); usual recycle ratios are between 2.3 and 6 [90]. The methanol is then separated from by-products such as water or dimethyl ether by distillation.

Methanol has a high-octane number and can be used directly as gasoline - with vehicle modifications. An admixture of up to 3% by volume of methanol is permissible in commercially available gasoline (according to DIN EN 228). Methanol has a significantly lower volumetric calorific value than fossil gasoline.

Table 22 provides an overview of methanol synthesis.

Table 22 Methanol synthesis fact sheet

Raw materials	Synthesis gas			
Products	Methanol → OK → (DK, Jet)			
By-products				
Yields	per pass: max. 25 % (> 95 % with loop control) energy efficiency: 75 % (without waste heat recovery)			
GHG emissions g CO2 eq/MJ		Standard (REDII)	typical (REDII)	model
	Cultured wood	14	14	4
	Waste wood	16	16	13
	Straw	k. A.	k. A.	6
	e-electricity	k. A.	k. A.	16
	e-Electricity +DAC	k. A.	k. A.	20

Downstream products from methanol

Methanol can not only be used directly, but also act as a platform chemical and starting material for the production of various downstream products (C1-Chemicals), some of which are also suitable for energy applications (see Fig. 39). For example, methanol can be converted via various processes (MtG, olefin oligomerization) into a product mixture whose properties can be specifically optimized for the application. Another important class of substances that can be produced from methanol are ethers. Dimethyl ethers and the substance class of oxymethylene ethers should be mentioned here. Methanol is also a reaction partner for the production of biodiesel and MTBE.

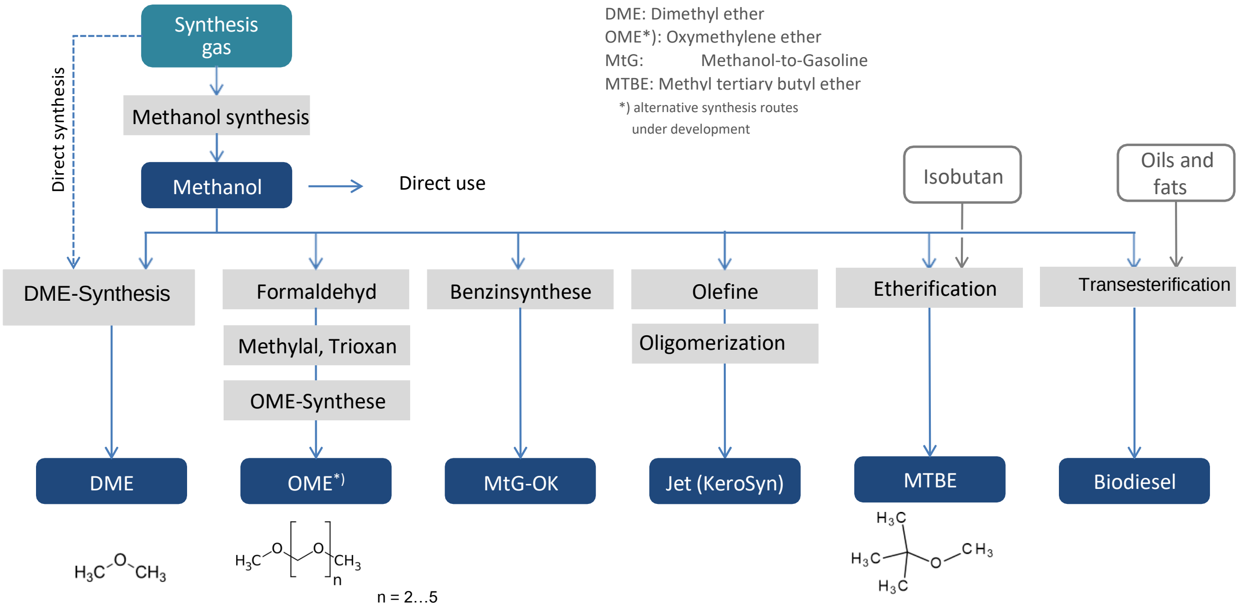


Figure 39 Process scheme for the production of methanol downstream products

Dimethyether

Dimethyl ether (DME), the simplest ether, is formed by etherification as a by-product in methanol synthesis. The targeted synthesis from methanol is carried out at temperatures of 250 °C to 400 °C and pressures of 10 to 25 bar on acid catalysts.

(20) DME synthesis from methanol: $2\ CH_3OH \rightarrow CH_3\text{-}O\text{-}CH_3 + H_2O$

DME is separated from the reaction mixture by distillation. The unreacted methanol can be recycled. Since the thermodynamic equilibrium is more on the side of DME, the cycle ratios are comparatively low.

Alternatively, DME can be obtained by direct synthesis from synthesis gas (H2:CO ratio 1:1)::

(21) DME synthesis from syngas: $3\ CO + 3\ H_2 \rightarrow CH_3\text{-}O\text{-}CH_3 + CO_2$

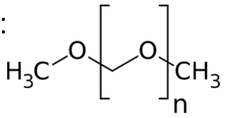
In principle, the water gas shift reaction, the methanol synthesis and the DME synthesis from the methanol produced in the process run simultaneously. Process control is largely the same as for methanol synthesis. Suitable catalysts are bifunctional copper-zinc catalysts on acid supports, which catalyze methanol synthesis via the metal function and DME synthesis via the acid function.

DME is gaseous at room temperature; with a vapor pressure of 6.9 bar at 30 °C, it can be stored as a liquefied gas in pressure vessels. It has good ignition properties (cetane number: 55) and is therefore suitable as a fuel for diesel engines. However, the use of DME requires, in addition to a test of material compatibility (especially of polymers), a certain modification of the tank and injection system in the vehicle, analogous to the conversion of OK vehicles to LPG. Since DME has no C-C bonds, it burns with very low soot [91].

Oxymethylene ether

Oxymethylene ethers (OME) are polyethers with a similar basic structure to DME. In their basic structure, carbon and oxygen atoms alternate. The oligomers preferred for use as diesel fuel due to their boiling point have a degree of oligomerization of 3 to 5.

Oxymethylene ether:



As with DME, there are no C-C compounds in OMEs, so they burn with very low soot [92]. Even as a blending component, OMEs reduce soot generation in diesel engines [92]. The calorific value of OME is significantly lower than that of fossil diesel fuel due to the oxygen content.

The material compatibility of polymers with OME is limited. The storage stability is lower than of fossil fuels, a small fraction of OMEs polymerize after prolonged storage, or split to form problematic shorter oxygenates, such as formaldehyde, formic acid, or methanol [93]. The lower storage stability mainly affects pure OMEs; as a blending component to conventional fuel oil or diesel fuel, OMEs appear to be stabilized by dilution [93]. OMEs are readily miscible with conventional diesel, but in paraffinic diesel (e.g., HVO), the two components segregate over a wide range of mixing ratios; here, biodiesel, for example, could serve as a solubilizer [94].

Currently, the synthesis of OME is relatively complex and proceeds via the intermediates formaldehyde, trioxane and methylal (trivial name for OME1). Formaldehyde synthesis via partial oxidation of methanol releases a not inconsiderable portion of the chemically bound energy of methanol, which is why the energy input for OME synthesis is higher than for other downstream products of methanol.

Methanol-to-Gasoline

In the methanol-to-gasoline (MtG) process, a synthetic gasoline substitute with almost ideal properties is produced from methanol in a single step. The reaction process can be described in simplified form using the following equations:

(22) Ether formation $2\ CH_3\text{-}OH \rightarrow CH_3\text{-}O\text{-}CH_3 + H_2O$

(23) Olefin formation $CH_3\text{-}O\text{-}CH_3 \rightarrow CH_2{=}CH_2 + H_2O$

$CH_2{=}CH_2 + CH_3\text{-}OH \rightarrow CH_2{=}CH\text{-}CH_3 + H_2O\ \ldots$

In further subsequent reactions (cyclization, dehydrogenation, methylation), naphthenes and aromatic components are formed. All of the methanol is converted. The strongly exothermic reaction is carried out at 310 to 430 °C and low pressures of about 5 bar on acid zeolites (ZSM-5) in adiabatic fixed-bed reactors or cooled shell-and-tube reactors [95]. During the reaction, the catalyst carbonizes and must be regenerated regularly. To ensure continuous operation, several reactors are usually used, which can be regenerated periodically in alternation (swing reactors).

The product is a mixture of hydrocarbons in the naphtha boiling range. Water and low-boiling hydrocarbons are formed as by-products. Table 23 compares typical properties of the gasoline fractions from two MtG processes. They differed only slightly.

Table 23 Octane numbers and composition of MtG crude gasoline of different MtG processes [95], [96]

Parameter		**STF[*] (CAC[**]/TU Freiberg)**	**MtG (ExxonMobil)**
ROZ		93 – 95	92
MOZ		84 – 85	82
Kerosenes	Vol.-%	58 – 66	53
Olefins	Vol.-%	4 – 5	12
Naphthenes	Vol.-%	6 – 9	9
Aromatics	Vol.-%	22 - 30	26
Benzene	Vol.-%	0,2 – 0,4	0,3
Durol	Vol.-%	bis 3	k. A.

[*] STF: Syngas-to-Fuel
[**] CAC: Chemieanlagenbau Chemnitz GmbH

Table 23 shows that the octane number of MtG crude gasoline is very close to the standard requirements for gasoline, and the aromatics and benzene contents also meet the requirements. It is excellently suited as a blending component and can be used directly as gasoline with minor processing. Only the relatively high content of durol (1,2,4,5-tetramethylbenzene) is problematic because of the high melting point of 79 °C. Therefore, hydrogenation of the heavy gasoline fraction may be necessary [96].

Olefin oligomerization

The double bonds contained in alkenes (olefins) provide the prerequisite for the assembly of several small molecules into a larger one (dimerization, oligomerization, polymerization). The choice of process conditions and the composition of the olefin mixture used can be used to control the product properties and thus produce "tailor-made" fuels. This is of particular interest for the production of alternative jet components that cannot otherwise be obtained with high selectivity. Similar to the alcohol-to-jet process (see 3.2.5), the products are highly branched aliphatic hydrocarbons with C numbers between 8 and 14. These are characterized by outstanding refrigeration properties.

As part of the "KeroSyn100" project, a demonstration plant is being planned at the Heide refinery in Schleswig-Holstein. Surplus electricity from wind farms and CO2 from a cement plant will first be converted into olefins (ethene, propene, butenes) via the intermediate methanol (MtO[12] process) and then oligomerized into high-quality jet fuel [97].

---

[12] MtO: Methanol-to-Olefins

Biodiesel

For the production of biodiesel, natural oils or fats are subjected to transesterification with methanol (see also section 3.2.2). In this respect, biodiesel can also be regarded as a downstream product of methanol. If non-fossil carbon is used for its extraction (BtL or PtL processes), the GHG footprint of biodiesel is reduced.

Methyl tert-butyl ether (MTBE)

MTBE is formed by a reaction of iso-butene with methanol. The exothermic reaction is acid catalyzed and is carried out in adiabatic fixed-bed reactors. Like ETBE[13], MTBE has outstanding anti-knock properties and is primarily added to premium fuels in proportions of 10 to 15% to improve the octane number.

Table 24 Fact sheet methanol downstream products

Raw materials	Synthesis gas				
Products		Dimethyl-ether (DME)	Oxymethylene-ether (OME)	OK (MtG-Process)	Jet, DK (Kero - Syn 100)
Yields	energy efficiency	80 %	54 %	64 %	Not modeled
By-products		-	-	Liquid gas	OK
GHG-emissions g CO2 eq./MJ	 Waste wood Cultivated wood Straw e-electricity e-Electricity (+DAC)	Model t4 (14*)) 1 2 (16*)) 5 15 17	Model 5 16 7 21 24	Model 4 13 5 16 19	Not modeled

*) Default values according to RED II

Methanization

Methanation is the hydrogenation of carbon oxides to methane. It is one of the first processes described for the use of synthesis gas but has hardly been applied on a large scale due to the availability of natural gas. The methanation of CO2 is also known as the Sabatier reaction. The reaction equations are:

(24) Methanation of CO: $CO + 3\,H_2 \leftrightarrows CH_4 + H_2O$

(25) Methanation of CO_2: $CO_2 + 4\,H_2 \leftrightarrows CH_4 + 2\,H_2O$

The strongly exothermic reaction is technically carried out at temperatures of 250 to 700 °C and an elevated pressure. Nickel is used as the active catalyst component. Adiabatic or cooled fixed-bed reactors can be used as reactors. In the case of using adiabatic reactors, a product stream is recycled to limit the heating of the reactor (see Figure 40). The carbon oxides are not completely converted in a reactor; the equilibrium is not completely on the side of the products.

---

[13] ETBE: Ethyl tert-butyl ether

To achieve higher conversions, several reactors are connected in series, and the equilibrium position is successively shifted toward methane by intermediate cooling and removal of the reaction product water. Of the processes considered here, methanation has the highest efficiency for the utilization of synthesis gas.

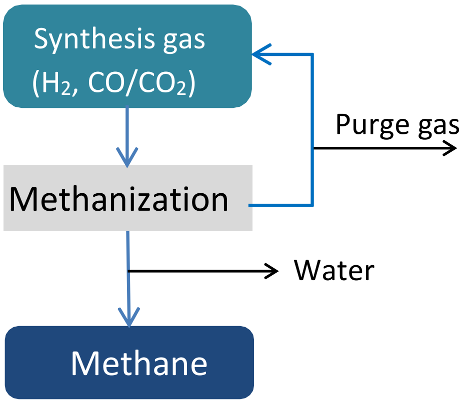


Figure 40 Process diagram methanation

Methane is the main component of natural gas. Synthetically produced methane has basically the same fields of application as natural gas; it can be used, for example, in gas burners for heat generation or as CNG[14] in natural gas vehicles.

The necessary infrastructure for transporting methane (gas grid) and storing it (cavern and pore storage) is already available. Another application, especially for PtG, would be its use as chemical energy storage for excess electricity.

In Table 25 is a fact sheet on methanation.

Table 25 Methanation profile

Raw materials	Synthesis gas: CO + H_2 respectively CO_2 + H_2		
Products	Methane		
By-products	None		
Yields	Energy efficiency:	BtG: 79 % (Without waste heat utilization) PtG: 85 % (Without waste heat utilization)	
GHG emissions		Standard (according to 37. BImSchV)	model
g CO2 eq/MJ	Cultured wood	k. A.	2
	Waste wood	k. A.	10
	Straw	k. A.	4
	e-electricity	3	13
	e-Electricity +DAC	k. A.	14

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[14] CNG: *compressed natural gas*

3.5. Interim conclusion

Conventional biofuels are comparatively easy to produce. Due to differences in their application properties, they can/should only be blended with conventional fuels to a limited extent. An exception is hydrogenated vegetable oils (HVO), which in principle cannot be distinguished chemically from conventional diesel fuel. The raw materials for conventional biofuels are generally cultivated biomasses, the potential uses of which are also politically limited (max. 4.4% for energy in Germany).

In principle, fuel syntheses allow the production of "tailor-made" products for all mobile applications. The intermediate product synthesis gas makes it possible to decouple reactant and product properties. The required synthesis gas can be obtained sustainably from biomass (residual wood, straw) or electricity-based from carbon dioxide and electrolysis hydrogen. While products can be obtained very selectively via methanol synthesis as individual components (methanol, MTBE, DME, OME) or mixtures (gasoline, jet), Fischer-Tropsch synthesis always delivers a broad product spectrum of predominantly paraffinic products.

Oxymethylene ethers (OME) have no direct carbon-carbon bond in their molecules and therefore burn particularly cleanly in diesel engines without soot formation. However, their production is costly and less efficient.

Figure 41 shows manufacturing costs for various products taken from literature data [8]. The price decrease with projection into the future is due to "learning effects" and "economies of scale".

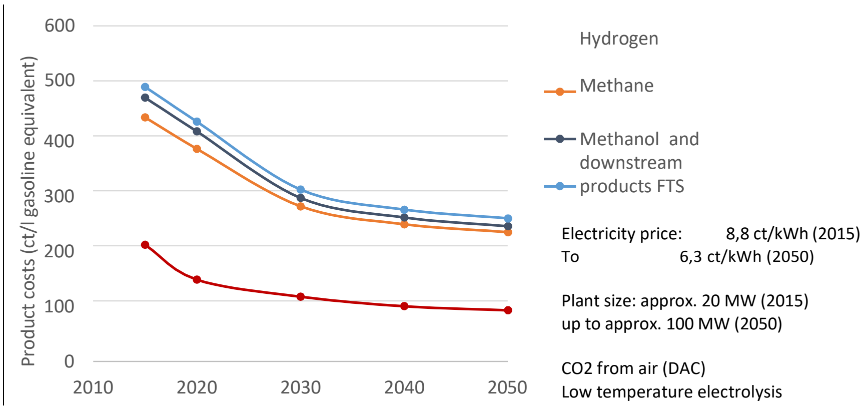


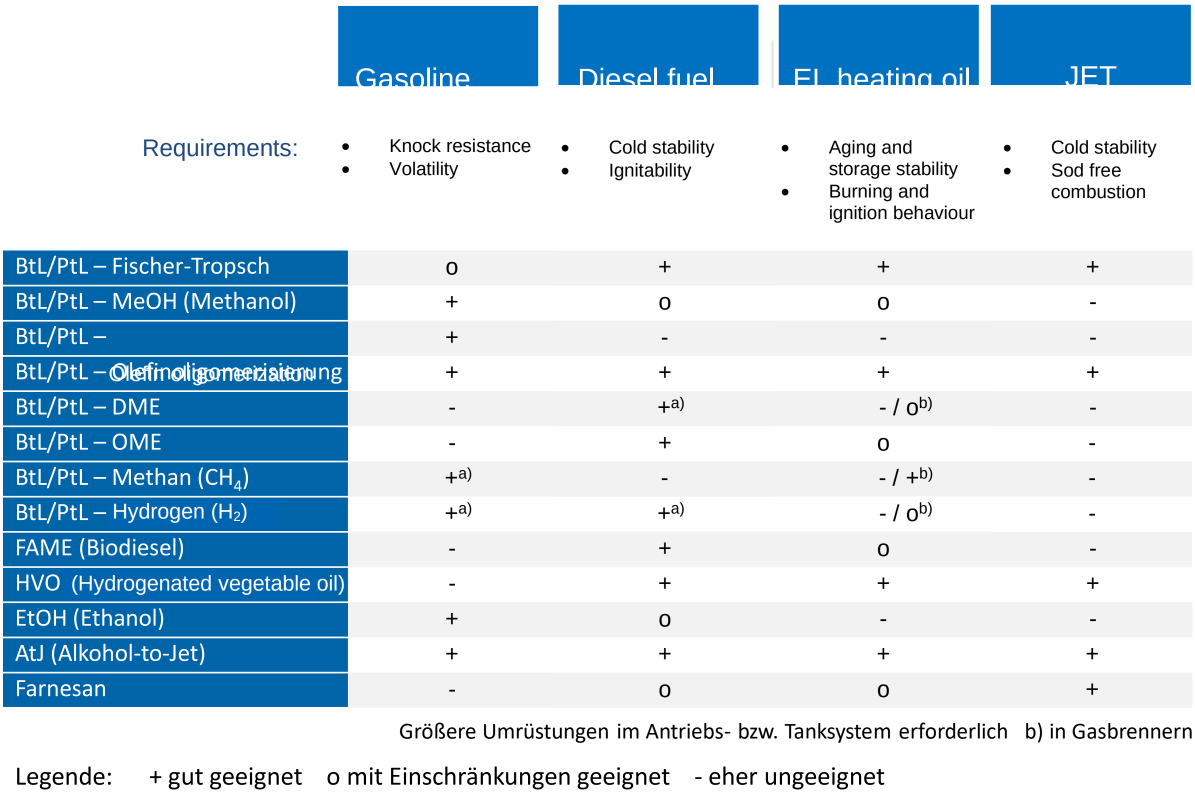
Figure 41 Product costs for synthetic fuels (from FVV report [8], costs for H2 calculated according to data in [8]).

As expected, hydrogen is the least expensive product. The other products can be produced at comparable prices, although methane production turns out to be slightly cheaper.

4.5. Products overview

The most important liquid final energy carriers, which to date have been produced predominantly from petroleum, include gasoline and diesel fuel, Jet A1 jet fuel, and light heating oil HEL. Very high and different requirements are placed on these products, so that not all the GHG-reduced fuels investigated are equally suitable for every area of application.

Figure 42 shows decisive properties for the target products mentioned, which are defined by their application. At the same time, the figure records important process chains or alternative products with a rough assessment of their suitability for substituting fossil energy sources for the various areas of application (+: well suited, o: suited with restrictions, -: rather unsuitable).



	Gasoline	Diesel fuel	EL heating oil	JET
Requirements:	• Knock resistance • Volatility	• Cold stability • Ignitability	• Aging and storage stability • Burning and ignition behaviour	• Cold stability • Sod free combustion
BtL/PtL – Fischer-Tropsch	o	+	+	+
BtL/PtL – MeOH (Methanol)	+	o	o	-
BtL/PtL –	+	-	-	-
BtL/PtL – Olefinoligomerisierung Olefin oligomerization	+	+	+	+
BtL/PtL – DME	-	+a)	- / ob)	-
BtL/PtL – OME	-	+	o	-
BtL/PtL – Methan (CH_4)	+a)	-	- / +b)	-
BtL/PtL – Hydrogen (H_2)	+a)	+a)	- / ob)	-
FAME (Biodiesel)	-	+	o	-
HVO (Hydrogenated vegetable oil)	-	+	+	+
EtOH (Ethanol)	+	o	-	-
AtJ (Alkohol-to-Jet)	+	+	+	+
Farnesan	-	o	o	+

Größere Umrüstungen im Antriebs- bzw. Tanksystem erforderlich b) in Gasbrennern

Legende: + gut geeignet o mit Einschränkungen geeignet - eher ungeeignet

Figure 42 Overview products and application areas

The resulting products are either

- Single substances or simple substance mixtures as drop-in admixture components,
- multi-substance mixtures as full-value fuels or blending components, or
- multi-substance mixtures or individual components as alternatives that are not drop-in-capable or only drop-in-capable to a limited extent.

The products considered are summarized in Table 26, arranged according to product or process groups.

Table 26 Products - Overview

	Process chain	product	use
Synthetic fuels • **- based on synthesis gas from biomass or electricity**	FT-Synthesis	Paraffine	OK, DK, HEL, Jet-Components
	MeOH-Synthesis • Syngas-to-Fuel (STF) [98] • DME-Synthesis • OME-Synthesis	Methanole/MTBE STF-Gasoline DME OMEs	OK-Components OK DK-Alternative DK-Components
	Olefin oligomerization [99] [88]	Isoalkane	Jet, Jet-Components
Fermentation-based fuels • **- from carbon hydrates (sugar, starch or cellulose)**	Alcoholic fermentation	Ethanol/ETBE	OK- Components
	ABE fermentation and condensation [100]	Isoalkane	Jet-, DK-, HEL-Components
	Fermentation with special yeast [60]	Farnesene/Farnesane	Jet-, DK-, HEL-Components
	Alcohol-to-Jet (AtJ) [101]	Isoalkane	Jet-, DK-, HEL-Components
Biogenic oil-based fuels • **- From lipids**		Vegetable oil	DK, HEL-Substitute
	Transesterification	Biodiesel/FAME	DK, HEL-Components
	hydrogenation/isomerization	HVO/HEFA1)	DK, HEL-(Components)
Upgraded products • **- From biomass**	reactive distillation [102] and Hydrogenation [59]	CVO, hydrogenated2)	DK, HEL-(Components)
	Hydrothermal liquefaction (HTL) and hydrogenation [103] [104]	Algae biocrude, hydrogenated	OK-, DK-, HEL-, Jet- Components
	TCR3) [105] + hydrogenation	Biocrude, hydrogenated	DK-, HEL-(Components)

1) HVO: Hydrogenated vegetable oils HEFA: Hydrogenated esters and fatty acids. en

2) CVO: Cracked Vegetable Oil

3) TCR: TCR: Thermal Catalytic Reforming

4) STF: Syngas-to-Fuel

4.6. Properties and drop-in capability

4.2.1. Petrol

The operating principle of gasoline engines places high demands on the properties of the fuels. To avoid uncontrolled or premature ignition ("knocking"), a high knock resistance, expressed by the octane number, is required. At the same time, an ignitable, vaporous fuel/air mixture must be present in the combustion chamber under all operating conditions (boiling range, vapor pressure). Table 27 lists the technical application properties of gasoline and fuel components.

Table 27 Petrol fuel and component properties

			Methanol	**Ethanol**	**1-Butanol**	**ETBE**	**MtG (STF)**	**FT-Gasoline**
RON		95	$106^{1)}$	$108^{1)}$	$94^{2)}$	117	93 – 95	<40
Heating value	MJ/l	32,0	15,4	21,2	26,8	26,9	≈ 32	
Fuel equivalent	l/l	1,0	0,48	0,66	0,84	0,84	≈ 1,0	
Density (15,5°C)	g/l	720 - 775	796	794	814	750	720 - 760	723
Aromatics content	Vol.-%	max. 35	keine	keine	keine	keine	22 - 30	<1
O-content	Ma-%	0 - 3,7	50	35	22	16	0	
Boiling temperature	°C	25 - 210	65	78	118	73	max. 210	35 - 200
Vapor pressure (37.8 °C)	kPa	< 60 (So) < 90 (Wi)	32	16	2,2	ca. 40	50 - 80	67
Solubility in water (20 °C)	g/100g	negligible	fully miscible	fully miscible		20,1	1,2 negligible	negligible

[1] OZ index for blending 130 [2] Isobutanol: RON 106

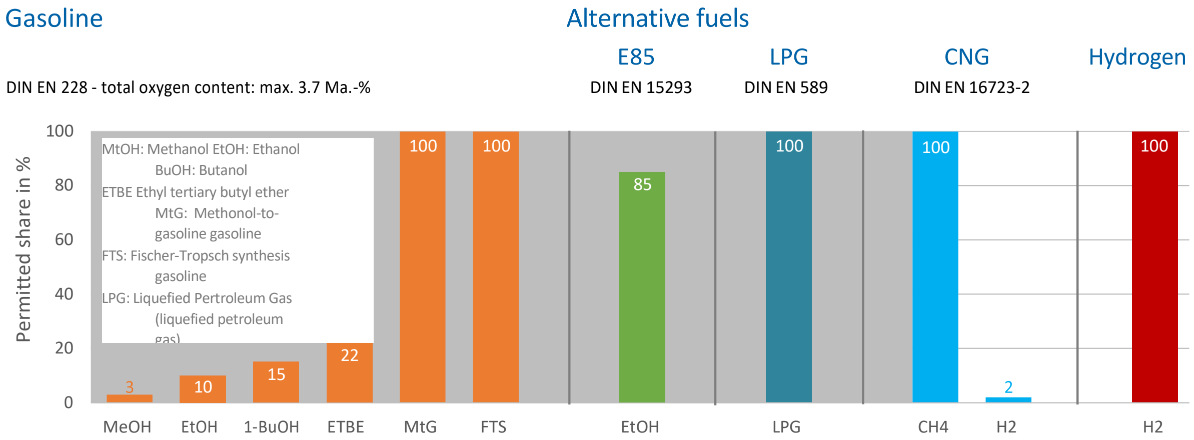
Many of the alternative gasoline fuels listed in Table 27 are single components with oxygenated functional groups (alcohols, ethers). These generally have good anti-knock properties (improvement in octane number). However, the oxygen content is associated with a reduced calorific value. The vapor pressure of the oxygenated components is sometimes lower than that of fossil gasoline, which can cause problems during cold starting. Other differences include the water affinity of most polar oxygenated components and a higher solubility compared to some polymeric materials.

MTG or STF gasolines are hydrocarbon blends with a high aromatics content and are characterized by excellent anti-knock properties. However, the crude products contain 1,2,3,5-tetramethylbenzene (trivial name: Durol), a substance with a high melting point, the content of which must be lowered for use as gasoline.

The Fischer-Tropsch synthesis leads primarily to linear, unbranched alkanes with a high tendency to knock. The gasoline fraction of the synthesis products therefore requires complex upgrading (hydro isomerization) to form antiknock branched kerosenes.

The liquid components listed in Table 27 can in principle be blended with conventional gasoline and are thus drop-in-capable. Limitations result from the fulfillment of the requirements according to DIN EN 228 [42]. Gaseous components such as methane, hydrogen and LPG are also suitable as gasoline fuels. However, this requires certain modifications, in particular the tank system must be designed for the higher pressures required. Only butane can be added to or dissolved in conventional gasoline; the vapor pressure specified by the standard must not be exceeded.

Figure 43 shows comparative blending limits for gasoline components and substitutes.



E85: Gasoline with 85 Vol.-% Ethanol

Figure 43 Drop-in capability of OK components and substitutes

According to DIN EN 228, the oxygen content is essentially relevant for the blendability of gasoline. The standard limits this to 2.7% by weight (for E5) and 3.7% by weight (for E10), so that this results in upper limits for blending components containing oxygen. Technically, higher percentages are possible. For example, the oxygen limit leads to a maximum methanol content of 3% by volume. In China, however, fuels with a relatively high methanol content (from coal gasification) are common [106]. For ethanol, a fuel with up to 85 vol.% ethanol is standardized, but this so-called E85 requires modifications to the vehicle.

In the case of synthetically produced gasoline from the Fischer-Tropsch synthesis or the product of the syngas-to-fuel (STF) or methanol-to-gasoline (MtG) process, there are no restrictions on the standard side, provided that compliance with the properties required by DIN EN 228 can be ensured by upgrading. This upgrading is costly in the case of Fischer-Tropsch gasoline, which consists largely of undisclosed kerosenes and olefins and therefore has far too low anti-knock properties. In comparison, STF gasoline already meets most of the requirements and needs only minor upgrading.

4.2.2. Diesel fuel

Diesel engines operate on the principle of self-ignition and therefore require fuels with a sufficiently high reactivity or ignition capability. One measure of this is the cetane number. In addition, cold resistance, i.e. flowability at low temperatures (cold filterability CFPP), is an important parameter for diesel fuels. Table 28 shows the application-related properties of diesel fuels and components.

Table 28 Properties of diesel fuel and components

					HVO/FTS	OME 4	DME
Cetane number (CZ)		> 51	36	54	>70	84	55
Calorific value	MJ/l	36,0	34,3	33,2	34,3	19,5	20,7
Fuel equivalent	l/l	1,0	0,95	0,92	0,95	0,54	0,58
Density (15,5°C)	g/l	820 – 845	916	870 - 900	770-790	1.083	740
Filterability (CFPP)	°C	-20 1)	N.measurable	-12	-5 – -25	-10	-141
Flash point	°C	min. 55	285	188	>61	88	-42
Viscosity (40°C)	mm²/s	2 – 4,5	30	3,5 - 5	2 – 4	1,75	0,19 3)
Boiling point	°C	200 – 360	Decomposition	321 - 350	200 - 320	202	-25

1) CFPP for winter diesel 2) Palm oil methyl ester: CZ: 62, CFPP: +13 °C

RME = rapeseed oil methyl ester DME = dimethyl ether

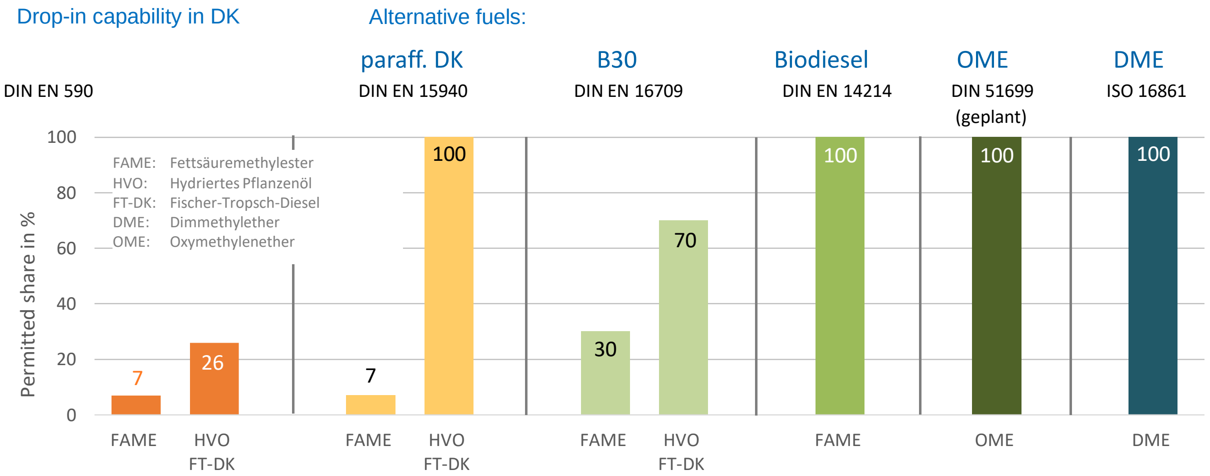
OME = oxymethyl ether HVO = hydrogenated vegetable oils

FTS = Fischer-Tropsch synthesis

Unprocessed vegetable oils (e.g. rapeseed oil) are unsuitable for use as diesel fuel without modifications to the vehicle due to their high viscosity. In contrast, methyl esters (biodiesel), which can be obtained by transesterification, have application properties that are comparable to conventional diesel fuels. The ester groups give the fuel its biodegradability. However, the oxygen bound in them also results in a somewhat lower energy content. The double bonds of the unsaturated fatty acid residues cause aging phenomena during storage. This can cause problems in systems where the fuel remains in the tank for a long time. Examples would be plug-in hybrid vehicles, which are rarely used for long distances, or vehicles that are only operated seasonally or periodically (motorboats, fire departments ...), for which biodiesel-free fuels are required.

HVO and the chemically very similar Fischer-Tropsch diesel contain practically no aromatics and consist essentially of kerosenes. These have good fuel properties such as excellent cetane number and high storage stability. However, their density is comparatively low, resulting in a somewhat lower volumetric calorific value. The primary longer-chain, unbranched alkanes tend to crystallize at low temperatures. Therefore, an isomerization step is necessary to achieve good low-temperature properties. The absence of aromatics can lead to problems. In vehicles that also run on conventional fuel, seals can swell or leak when operated with purely paraffinic fuels [27].

Other diesel fuel substitutes are dimethyl ether (DME) and the homologous series of oxymethylene ethers (OME) based on it. They contain no C-C bonds and therefore burn almost soot-free. Diesel engines with adapted engine management can thus be operated with virtually no emissions, and the cost of exhaust gas aftertreatment could be significantly reduced. As a result of the high oxygen content, OME and DME have a greatly reduced energy content. The strongly differing solubility and swelling properties of OME are problematic. DME, on the other hand, is a liquid gas and requires similar vehicle adaptations as the use of LPG for gasoline engines.



B30: Diesel fuel with 30% by volume FAME

Figure 44 Drop-in capability of DK components and substitutes

Figure 44 shows a comparison of the blending limits and drop-in capability of various diesel substitutes. For biodiesel (FAME), the fuel standard specifies a maximum proportion of 7% by volume. The background to this is the water affinity caused by the ester groups and the associated microbiological changes, as well as the biodiesel penetration into the engine oil. In contrast, the addition of paraffinic products (HVO, FT diesel) is not explicitly restricted. However, the fulfillment of the lower density limit according to DIN EN 590 [41] results in a practical limitation, which is about 26% by volume. OMEs are not compatible with current diesel fuel according to DIN EN 590 due to their solubility and swelling properties.

4.2.3. Jet-Fuel

The special conditions of aviation place the highest demands on the fuels used:

- Resistance to cold and high temperatures (no kerosene precipitation, good pumpability, no ice formation, no vapor formation)
- Purity (residue-free combustion -> turbine damage)
- High thermal value (long range)

In addition, for safety reasons, alternative jet fuels must undergo a special approval procedure. Table 29 shows the properties of possible alternative fuel components compared with the requirements for Jet A1 (commercial aviation turbine fuel) according to ASTM D1655. Almost without exception, the currently approved alternative jet fuels are paraffinic fuels. These generally have a slightly lower density than required for Jet A1. However, the calorific value by mass is higher than for fossil jet. The refrigeration properties can be set to relatively low values.

Table 29 Jet fuel and component properties

		FT-Jet*)	AtJ	Farnesan
Heating value MJ/kg	> 42,8	n. b.		44,2
Density (15,5°C) g/l	775 - 840	743 - 755	757	774
Soot point mm	25	n. b.	>>25	>>25
Freezing Point °C	< -47	-43		< -75
Aromatics content Vol.- %	> 25	None	None	None
Viscosity (-20 °C) mm²/s	< 8	3,5		
Flash point °C	> 38	42	49	109
10 % Evaporates °C	< 205	140	175	247
to boiling point °C	< 300	280	250	

*) own studies AtJ = Alcohol-to-Jet

The drop-in capability of GHG-reduced jet fuels is regulated by ASTM D7566. It should be noted that not only the properties and composition of the individual fuels are important, but also the origin in terms of the general production principle. Currently, Fischer-Tropsch kerosene, HVO, AtJ from isobutanol, as well as farnesane are approved as alternative jet fuels, but only up to a maximum of 50% by volume depending on the fuel (Figure 45).

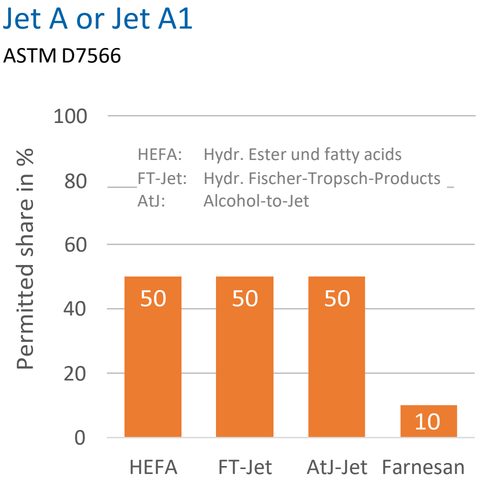


Figure 45 Drop-in capability of jet components

4.2.4. Heating oil extra light (HEL) and gas

Although the share of gas and oil heating systems in new residential construction has decreased significantly in recent years (2020: 33.7 % gas heating, oil hardly plays a role anymore), the housing stock is still dominated by these heating systems (2020: almost 50 % gas, 25 % oil) [107]. Substituting fossil fuels with products with low GHG footprints can therefore make a significant contribution to reducing GHG emissions in the buildings field of action.

The fuel gas supplied to the consumer via gas grids consists of very high proportions of methane (95 to 99% by volume). Thus, both synthetically produced methane (SNG) and methane obtained after processing in biogas plants can be used for the substitution of natural gas. There is practically no limit to the amount of methane that can be blended. However, compliance with relevant parameters (e.g., calorific value or Wobbe number) must be ensured. Under this condition, hydrogen produced from renewable energy can also be fed into the natural gas grid in limited quantities. This also provides an opportunity for (chemical) storage of fluctuating so-called surplus electricity.

EL heating oil (extra-light) has similar properties to conventional diesel fuel, so that in principle the same alternative products can be considered as substitutes. Table 30 compares the requirements for extra-light heating oil according to DIN 51603/1 and the properties of the possible alternatives. Due to their much too high viscosity, non-esterified vegetable oils are just as unsuitable for the application as the liquid gas DME.

Table 30 Properties of heating oil extra light and heating oil substitutes

				HVO/FTS
Heating value MJ/kg	> 42,6	37,4	37,7	44,0
Fuel l/l equivalent kg/kg	1,0 1,0	0,95 0,88	0,92 0,88	0,95 1,03
Density (15,5°C) g/l	< 0,860	916	870 - 900	770-790
Solidification point °C Cloud point	< -6 < 3	n. measurable	-12$^{1)}$	-5 – -25$^{1)}$
Flash point °C	min. 55			
Viscosity (20 °C) mm²/s	< 6	285	188	>61
Boiling point °C	200 – 360	30	3,5 - 5	2 – 4
		Decomposition	321 - 350	200 - 320

$^{1)}$ CFPP (lies between solidification point and cloud point)

In contrast to vehicle applications, oil heating systems are characterized by a significantly longer storage time of the fuel in the storage tanks. Therefore, the specific properties of fatty acid methyl esters (FAME, e.g., RME) are of great importance and hinder an application as a substitute for light heating oil. The water affinity due to the ester groupings favors hydrolysis and thus a limited storability of heating oil containing FAME. Therefore, FAME in EL fuel oil is only tolerated as contamination up to 0.5% by volume. In contrast to fatty acid methyl esters, paraffinic substitutes, which can be produced, for example, by hydrogenation of vegetable oils (HVO) or by Fischer-Tropsch synthesis from synthesis gas, do not cause any stability problems and have outstanding combustion properties (see also Table 30). However, the absence of aromatic components can lead to failure of the flame retardant in burners due to insufficient flame coloration [108]. For this reason, among others, the minimum density of paraffinic products that can be added to EL heating oil is limited to approx. 50% by volume by the new version of DIN 51603/1 published in 2020. The use of biogenic components as heating oil is regulated in DIN SPEC 51603/6 (heating oil EL A Bio).

The drop-in capability or ad miscibility of alternative components to liquid and gaseous fuels is shown in Figure 46.

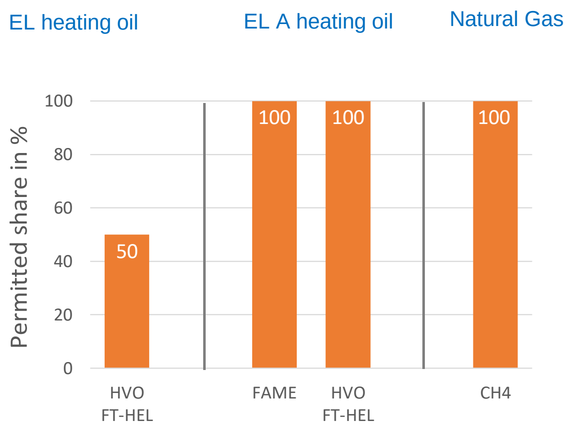


Figure 46 Drop-in capability of fuel oil components and substitutes or natural gas substitutes.

4.7. Interim conclusion

The GHG-reduced fuels and combustibles that can be produced from different raw materials and via different routes are well or very well suited substitutes for conventional products. However, their properties differ in part from those of the fossil reference. This often results in only limited blending capability with standard fuels. In some cases, the use of alternative products requires conversion measures on the vehicle (material compatibility, quantity metering, preheating, engine control, for gaseous alternatives: tank systems, metering, exhaust catalyst concepts). Some of the existing products that allow higher blends are currently hardly offered to end consumers in Germany (e.g., paraffinic diesel fuel, gasoline with 85% ethanol - E85). In some respects, GHG-reduced fuels may be superior to conventional fossil options, e.g., octane number for oxygenates, cetane number of paraffinic diesel fuels (HVO, Fischer-Tropsch), cold resistance of highly branched hydrocarbons (AtJ, farnesane, olefin oligomers). Moreover, the product properties of synthetic fuels (Fischer-Tropsch synthesis, oligomerization of olefins) can in some cases be very specifically adjusted.

In order to reduce greenhouse gas emissions in aviation, there are - apart from efficiency improvements and reduction of air traffic - no recognizable alternatives to the production of synthetic products. Their production often results in co-products (gasoline, gasoil), the use of which as power or fuel is indicated and sensible.

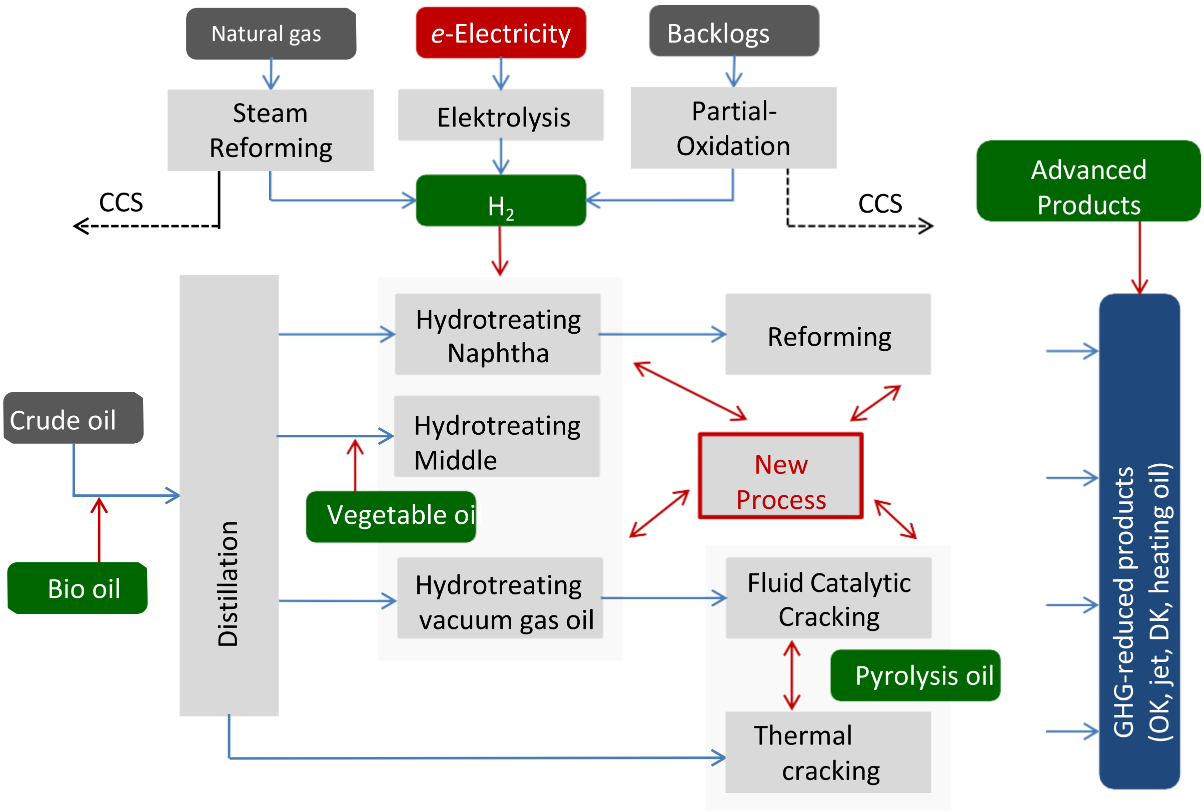
The production of electricity-based synthetic products has only low energy efficiency. However, this criterion is of secondary importance if sufficient "surplus electricity" or inexpensive electricity is available in the future. For imported products, the ease of transport of liquid products is also relevant.

5. Integrability into existing processes or plants

5.1. Integration of TGH-reduced substances in refineries

Petroleum refineries have numerous process plants to convert the multi-component mixture of crude oil into standard-compliant finished products. These include plants for separating the raw material into individual fractions as well as chemical conversion stages for adjusting the required technical application properties. In addition, there is an extensive infrastructure for the provision of other feedstocks and energy (e.g. hydrogen, steam, electricity), for the treatment and processing of by-products and residues (refinery gas, wastewater, residues, etc.), for the adjustment of application properties and standardized parameters (blending), and finally for the distribution of sales products. The configuration of refineries is characterized by a certain flexibility to accommodate variations in feedstock properties or changes in market requirements (type, quantity, and quality of products). The products are usually blended products from material streams of different process stages. In the so-called blending process, the finished product properties are specifically adjusted by mixing the various components.

Refineries are thus in an excellent position to integrate alternative materials and energy flows and thus reduce the GHG footprint of the finished products. At the same time, the existing distribution channels ensure the marketing of the products. Figure 47 shows various options for reducing greenhouse gas emissions in the production of fuels.



① Supply of green/blue hydrogen
② Co-Processing of vegetable oil
③ Substitution of fossil crude oil by biogenic feedstocks
④ Use of pyrolysis oils as co-feed during cracking
⑤ Exploitation of synergies in the production of advanced fuels
⑥ Blending

Figure 47 Possibilities for integrating alternative material flows in refineries

5.1.1. Use of green and possibly blue hydrogen

Hydrogen is one of the most important auxiliary materials in refineries, and its demand has increased sharply in recent decades. The reasons for this are stricter environmental standards for finished products (e.g. lowering of the permissible sulfur content in fuels and heating oils) and the increasing conversion of heavy components and the associated hydrogen deficit in the unsaturated cracking products. In the processing of crude oil, only the catalytic reforming of naphtha produces a significant amount of hydrogen, which can then be used for hydrogenations. The additional demand (about 136 kt/a in German refineries [109]) is currently largely met either by steam reforming of natural gas or partial oxidation of heavy residues. Substituting this "gray" hydrogen with so-called "green" hydrogen can significantly reduce GHG emissions from refineries. At the same time, this option offers a possibility to store fluctuating electrical energy from renewable sources.

If a defined amount of available green hydrogen is assumed, a comparatively larger GHG reduction can be achieved when used as hydrogenator H2 in refineries than in the production of synthetic fuels (PtL). The greatest effect is achieved with direct use, e.g. in fuel cells (Figure 48).

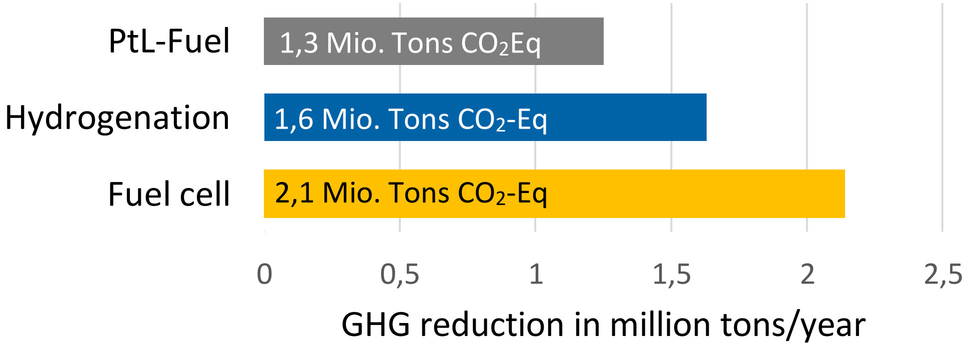


Figure 48 Comparison of GHG reductions achievable with "green" hydrogen (baseline: 136 kt/a H_2)

The use of green H2 in refineries can be credited with double the amount for meeting the GHG reduction quota (REDII) in the transportation sector [110]. Nevertheless, the leverage for meeting the GHG quota remains small. Even with a complete conversion to renewable hydrogen, the CO2 savings only correspond to an absolute share in the quota fulfillment of approx. 0.5 % (with double crediting: 1.0 %).

The production of green hydrogen is significantly more cost-intensive than the production of gray hydrogen, not least due to the high cost of electricity. However, the provision of hydrogen accounts for only a small part of the manufacturing costs of the finished products. In addition, sales prices are largely determined by taxes and duties. The conversion to green hydrogen is therefore only associated with a moderate increase in product prices and is particularly suitable for Germany for regional use at model locations or model regions.

Within the REFHYNE project, Shell operates a pilot plant at the Rheinland refinery in Wesseling (electrolyzer capacity 10 MW for 1,300 t H2/a) [111]. In another project (GET H2 Nucleus), RWE and BP are planning to build a 100 MW electrolyzer to produce green hydrogen and its use in the Lingen and Gelsenkirchen refineries [112], [113].

Provided that permanent storage of carbon dioxide is politically accepted and legally permitted as an option to reduce GHG emissions, existing H2 production technologies coupled with "carbon capture and storage" (CCS) could also be used to reduce the carbon footprint of conventional fuels (use of "blue" hydrogen).

5.1.2. Hydrogenation or co-hydrogenation of recent oils

Hydrogenation of recent oils (vegetable oils, used edible fats) can produce fuels with outstanding application properties (see also sections 3.2 and 4.2.2). The conversion requires similar reaction conditions (pressure, temperature, catalyst) as the hydro-refining of straight-run gas oils to produce low-sulfur middle distillates (diesel fuel, EL heating oil). Therefore, joint processing (co-processing) in refineries is an obvious option. Investigations in pilot plants showed that blending rates of up to 20% can be realized without major technical modifications [114], [115]. The vegetable oil can be blended directly upstream of the hydrogenation reactors. The product obtained is a desulfurized gas oil with the corresponding bio-fractions (HVO) as a mixture.

Joint processing leads to low investment costs and allows the use of synergies (provision of H2, gas purification, wastewater treatment, etc.). While the first plants were built as stand-alone plants, partly in the vicinity of refineries, co-processing is increasingly coming into focus as a suitable and favorable way to reduce CO2 emissions. However, in Germany, biogenic oils that are co-hydrogenated with mineral-derived oils in a refinery-based process cannot be counted toward meeting GHG emission reduction obligations (compared to a reference fuel) under the BImschG. The draft law for the further development of the GHG reduction quota of 12.02.2021 also does not provide for any changes in this regard.

At the beginning of 2020, production plants for HVO[15] with a capacity of 5 million tons per year were in operation in Europe, of which 0.42 million tons /a via co-processing) [116]

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[15] HVO: Hydrotreated Vegetable Oil

5.1.3. Substitution of fossil crude oil (Co-Feeding)

One possible way to obtain liquid energy sources is the so-called "direct liquefaction" of biomass. In this process, organic feedstocks are converted via thermal processes (e.g. pyrolysis, hydrothermal liquefaction) with the formation of by-products into liquid, oil-like products with a mostly broad boiling spectrum. These are generally very unsaturated and contain high proportions of undesirable hetero compounds that interfere with their application. They therefore require very complex upgrading by hydrogenation and cracking processes, which are also used in the processing of mineral oil. Particularly in the case of very high heteroatom contents, this is also associated with a very strong change in the molecular sizes and thus the boiling point (see Fig. 49). Local, decentralized processing into different finished products according to the boiling point of the individual fractions is not economically or technically feasible.

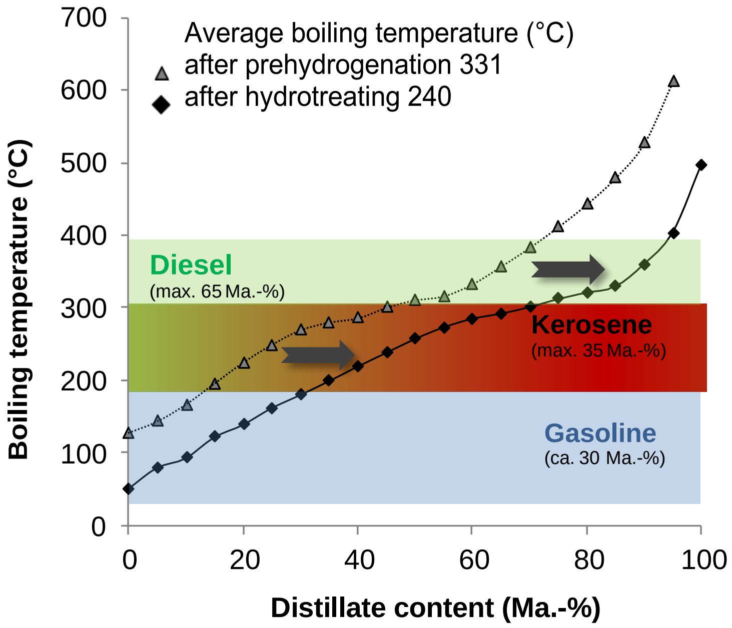

Figure 49 Boiling behavior of algal-derived products before and after hydrogenation [117]

However, such bio-oils could in principle be fed into the refinery process as biocrude prior to distillation and then, together with petroleum-derived components, undergo all the necessary steps to obtain standard-compliant sales products (fractionation, conversion, product-specific upgrading). An important prerequisite is that the co-processing of the biocrude does not lead to operational problems (coking, catalyst poisoning) and that the boiling behavior of the substances does not change significantly during their hydro refining. To convert the primary liquefaction products into a "refinery-ready" feedstock, prehydrogenation is therefore necessary, which could be carried out either decentrally at the bio-oil production site or centrally in a refinery before blending with the crude oil (see Fig. 50). During this prehydrogenation, a large part of the hetero compounds is already converted, so that the change in boiling point associated with hydro refining in the refinery can be tolerated.

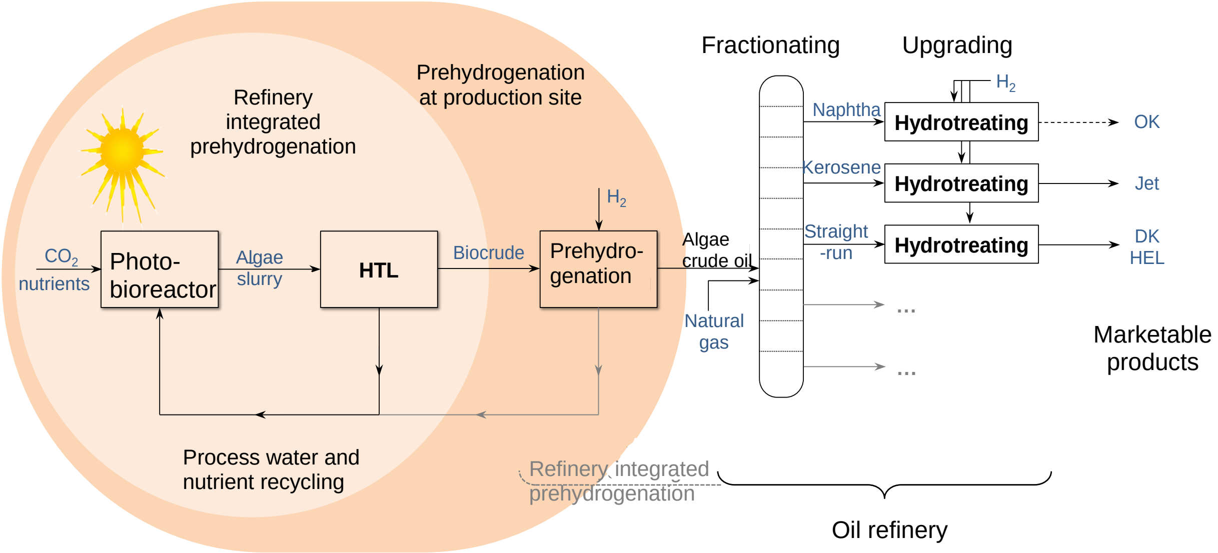

Figure 50 Schematic of a co-processing of pre-hydrogenated bio-oils (e.g. algal crude oil, HTL hydrothermal liquefaction) in a refinery [117].

5.1.4. Co-processing of pyrolysis products during the cracking of high-boiling ingredients and/or residues

In refineries, thermal or catalytic cracking processes are used to convert high molecular weight petroleum components into additional low-boiling products such as naphtha and middle distillates. Particularly in thermal processes that can process distillation residues, there is in principle the possibility of co-processing also biogenic and possibly viscous pyrolysis products with high proportions of heteroelements. The resulting low-molecular-weight biogenic and petroleum-derived fission products can be processed together into finished products in the existing plants according to their boiling point.

In contrast, catalytic processes such as fluid catalytic cracking (FCC) are suitable for the conversion of refined (hydrogenated) vacuum gas oils. Target products include gasoline and middle distillate components as well as valuable short-chain olefins (i-butene). The zeolitic catalysts used in this process are subject to deactivation by carbon deposits. In addition, polar nitrogen and sulfur compounds are adsorbed on the active centers of the catalysts, leading to immediate but temporary poisoning. The deactivation of the catalysts is counteracted by immediate and continuous regeneration. The requirements for the feedstocks are thus comparatively low. Permanent catalyst damage, on the other hand, is caused by heavy metals, which are contained in particular in petroleum-derived distillation residues.

Wood pyrolysis oils are generally very rich in oxygen functional groups but have only low nitrogen and sulfur contents. Their basic suitability for co-processing in the FCC process has been demonstrated by experimental studies [118]. Co-processing with a bio-oil content of 5% resulted in a slightly higher middle distillate yield and somewhat lower gaseous hydrocarbons. Most of the oxygen contained in the wood pyrolysis oil is split off in the form of carbon oxides and water. The amount of phenolic components in the product increases.

In addition to biogenic feedstocks, heavy oils from thermal-chemical plastics recycling can also be co-processed in the FCC process. In the so-called ReOil process of OMV [119], [120], plastic packaging waste is depolymerized. While the light product fractions are used again to obtain olefins for the chemical industry, the heavy oil fraction can be catalytically processed into valuable products in proportions of up to 20 % [121].

5.1.5. Utilization of synergies

With their excellent infrastructure, petroleum refineries also offer themselves as production sites for alternative fuels with a low GHG footprint (PtL and BtL products) but also for the chemical recycling of used plastics and organic waste. For so-called annex plants, there is the possibility to use numerous synergies and thus to reduce manufacturing costs:

- Provision of auxiliary materials (steam, boiler feed water, electricity) and hydrogen,
- Treatment and processing of auxiliary and residual materials (wastewater, gas purification, ...),
- distribution of finished products,
- safety engineering, blow-down and flare system.

In addition, the product properties can be specifically adjusted regarding product blending and subsequent use (tailor-made fuel). This also results in advantages for normal refinery operations.

5.1.6. Blending

In the various process plants of a refinery, product components are produced which, although they exhibit similar boiling behavior, can differ considerably in some cases in their other physical, chemical and application properties. For the production of standard-compliant sales products, these individual components are mixed in appropriate proportions (blending). It is important that the blended product meets the desired or required properties, while the individual components may well be outside the standard. In addition to the properties, the current market situation, production planning data or stock levels are also taken into account when determining the suitable formulations.

In addition, the blending process is also used to blend in imported products, i.e. products not produced in the refinery. This concerns both substances that help to improve properties and are therefore required (e.g., additives, MTBE or ETBE) and alternative fuel components (e.g., bioethanol, FAME, HVO), which are used by refineries to meet their obligations to meet GHG reduction quotas. Key advantages of blending in third-party products include the ability to use existing transportation and distribution channels, as well as quality assurance to consumers.

5.2. Interim conclusion

Refineries have a wide range of interconnected technologies for the production of standardized fuels (separation, chemical conversion and refining). Their infrastructure makes them ideal locations to produce alternative products (provision of raw and auxiliary materials, water and gas treatment, distribution). The existing plant technology can in principle be used for some of the required conversions.

The CO2 footprint of conventional products can be reduced by various measures:

- Incorporation of green or possibly blue H_2,
- Partial substitution of petroleum with pre-treated bio-oils,
- input and co-processing of alternative oils (co-processing):
  - synthetic crude products (e.g. Fischer-Tropsch products),
  - reclaimed oils and fats (vegetable oils, used cooking oils),
  - Pyrolysis products, recycled products,
- Incorporation of imported products.

By mixing individual material streams to form the finished product in the blending process, the product properties can be specifically adjusted. Alternative products (synthetic products, HVO) exceed the required values in some parameters and thus support the production of standard-compliant fuels. At the same time, the blending process and distribution via the refinery ensures the quality of the alternative products placed on the market.

Last but not least, security of supply is always ensured by gradually increasing substitution of fossil mineral oil by alternative input materials.

6. Process modeling and cost estimation

6.1. Methodology and Framework

The aim of the modeling was to enable a comparable estimation of the necessary costs for the production of GHG-reduced fuels. To this end, as also shown in Figure 51, the individual process steps were mapped in Aspen Plus at a medium level of complexity (as simple as possible and as detailed as necessary). The focus was to generate results that are readily comparable with each other using a uniform methodology. On the other hand, this also means that no intensive optimization of the individual process steps could be carried out.

The energy and material flows determined in the process modules were linked together for the overall process. Heat integration is achieved by coupling the heat flows (generation and demand) at the appropriate temperature levels. As a result, the total yield of the process, including the by-products, is obtained for the raw and auxiliary materials used in each case. In addition, the energy demand or generation is obtained. This includes the cooling requirement, if applicable. The operating costs can already be largely derived from these variables.

For the determination of the capital costs, a literature search was used, which provided a range of known or estimated capital costs for the individual process steps. In general, the capital costs used for the model were set approximately in the middle of this range. In the case of technologies that are not yet widely available on the market, capital costs that were assumed to have a certain learning curve were taken from the literature.

The capital and operating costs were then used to determine a product price according to standard methodology.

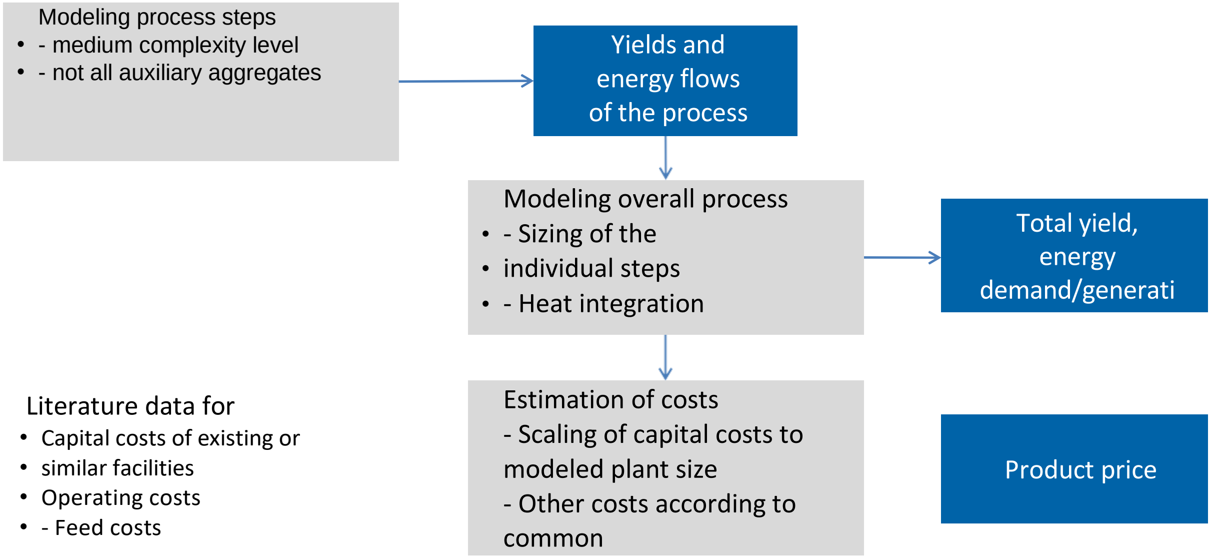

Figure 51 Modeling methodology

6.2. Cost calculation

6.2.1. Basic assumptions and methodology

The product prices necessary to cover the required capital and operating costs are determined using the terminal value method. Framework conditions for the estimation are:

- Equity ratio: 40 %
- Imputed interest rate: 10 %
- Repayment: after 10 years
- Return on investment: 10 %
- Inflation rate: 2 % (for labor costs: 3 %)
- Insurance: 1 % of the investment costs
- Taxes: 3 % of the investment costs
- Lifetime: 20 a
- Plant size: 100,000 t/a (gasoline equivalent)
- Reference year: 2018

For the terminal value method, the income and expenses (including equity) incurred in the respective annual slices are converted to their respective value at the end of the asset's life, the so-called terminal value, taking into account the rate of return.

$$EW = d \cdot (i + 1)^{n-t} \tag{26}$$

d …..Value of revenue/expenditure occurring in year t
n …..Lifetime of the asset in years
t ……year for revenue/expenditure, year 1 start-up, year n lifetime, equity in year 0
i ……imputed interest rate
EW ..Final value

The product price for which the summed final values of expenses and revenues match is the minimum selling price to generate the assumed rate of return.

6.2.2. Capital costs

For the sub-processes considered, data on the capital costs of existing or similar plants are taken from the literature. Since these data are usually not available for the necessary size of the steps considered in the process, a conversion must be made according to the following equation.

$$C_n = C \left(\frac{R_n}{R}\right)^{\chi} f_{CEPCI} \tag{27}$$

The capital costs Cn of the new plant are determined from the capital costs C of the known plant and the ratio of the capacities Rn and R of the new or known plant. This ratio also includes a degression coefficient χ, which takes into account the fact that the construction of a larger plant is specifically less expensive. Using the factor fCEPCI determined from the CEPCI price index [122], the researched costs from the respective reference year can be converted to the costs at approximately the present time (year 2018). It should be noted that capital costs given in the literature may refer to different project stages:

- Total Purchased Equipment Cost (TPEC).
- Total Installed Cost (TIC), which also includes the cost of installing equipment, including instrumentation, controls, piping, and the cost of land and buildings used.
- Total Project Investment (TPI) includes the total capital cost of a project. In addition to the TIC, the costs for engineering, construction, legal department, and subcontractors are included, and a safety margin is also calculated.

The conversion factors are in a certain range. According to [123], the TPI is typically 1.39 times the TIC and 3.43 times the TPEC. According to [124], there is a wider range, mean values for conversion factors from TIC to TPI are 1.6 and for TPEC to TPI are 4.8. The latter values were used in the modeling as conversion factors for literature data of capital costs. A learning curve was included in determining capital costs for processes that are not currently in large-scale industrial use. The capital costs used are intended to represent the costs after the technology has been largely established.

6.2.3. Operating costs

The running costs consist of costs for:

- Input (e.g., biomass),
- Electricity, heat,
- Other operating materials (e.g., catalysts),
- Maintenance and consumables,
- Labor costs.

Annual costs for maintenance and consumables are calculated as a flat rate of 7.0 % and 1.05 % of the capital costs of the plant [125]. The labor costs incurred can be determined on the basis of empirical values for the labor hours [125] and average labor costs [126] required per unit for certain production capacities. Administrative activities are added at a rate of 20 %..

The following values were assumed in the base case:

- Electricity: 50 €/MWh (Germany) or 20 €/MWh (MENA - PtL).
- Heat: from heat integration, possibly from electricity.
- Biomass (wood): 18 €/MWh (=88 €/tTM) [127]
- Wastewater disposal: 2.5 €/t [128]
- Pure water: 2 €/t [128]
- Cooling water: 0.09 €/t [129]
- Sale of electricity: 50 €/MWh
- Sale of heat: 20 €/MWh
- CO2 from point source: 30 €/t CO2 [130]
- Labor costs: 40,2 €/h [126]

Annual operating hours were assumed to be 8000 h/a. For electrolysers, 3000 h/a were assumed in the base case, assuming that the cheap necessary renewable electricity is not available all year round.

6.2.4. Definition of scenarios for different production sites

The supply costs for alternative fuels are also determined to a large extent by the framework conditions, which can differ substantially for different regions. Figure 52 shows the production locations considered in the study.

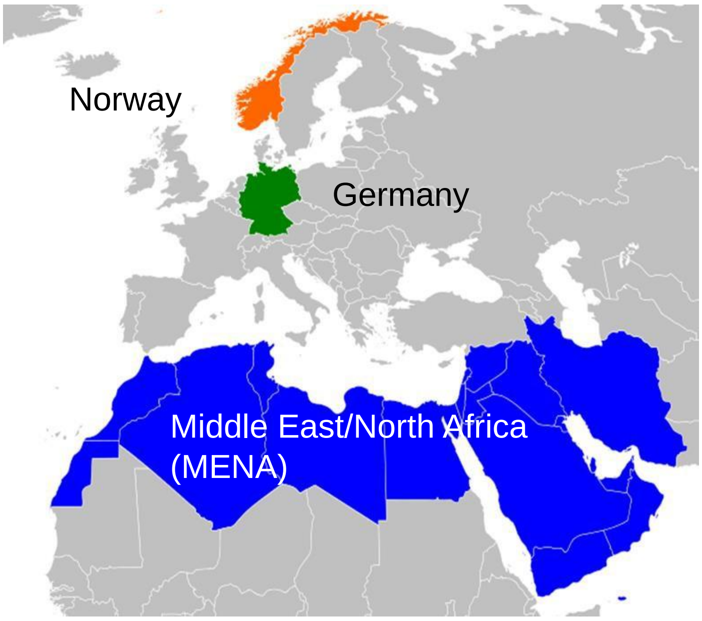

Figure 52 Production sites considered

The assumptions used for the modeling are summarized in the following tables.

Table 31 General conditions for Germany

Germany	
General	Biomass available CO2 point sources usable Operating time syntheses 8,000 h/a Operating time electrolysis 3,000 h/a
Cost of raw materials and supplies	Electricity: 5 ct/kWh Pure water: 2 €/t
Revenues	Electricity: 50 €/MWh District heating: 20 €/MWh Oxygen: 23,7 €/t
Transport	Distribution 500 km (Truck, distribution network)

For Germany (Table 31), a price for renewable electricity of 5 ct/kWh, which is available for 3,000 hours per year has been assumed. These costs are in the lower range of the range for electricity production costs[16] for onshore wind power in Germany [131].

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[16] It is assumed that PtL plants are not connected to the power grid, but directly to the, renewable power generating, plants.

Furthermore, it is assumed that both biomass and CO2 point sources are present.

Table 32 General conditions for Norway

Norway	
General	Biomass available CO2 point sources usable Operating time syntheses 8,000 h/a Operating time electrolysis **8.000 h/a**
Cost of raw materials and supplies	Electricity: **3 ct/kWh** Pure water: 2 €/t
Revenues	Electricity: **20 €/MWh** District heating: 10 €/MWh Oxygen: 23,7 €/t
Transport	To G **800 km** (Truck, Pipeline) Distribution 500 km (Truck, distribution network)

For Norway (Table 32), an electricity price of 3 ct/kWh was assumed for hydropower, which is in the lower range of the range of electricity production costs according to [132] and slightly above the favorable assumptions of 2.5 ct/kWh according to [133]. This electricity is available for most of the year. The use of point sources of CO2 is possible at this site, likewise biomass can be used. The transport distance to Germany is estimated to be about 800 km. The favorable price for renewably generated electricity, well-developed infrastructure, and the presence of point sources of CO2, as well as geographical proximity, mean that Norway has ideal conditions for electricity-based synthetic fuels. For example, one of the currently largest planned PtL pilot projects (Nordic Blue Crude together with Sunfire) [134], which is expected to produce 8,000 t/a of fuel, will be located in Norway.

Table 33 Framework conditions for the MENA region

MENA	
General	Biomass not available CO2 capture air, alternatively point sources usable Operating time syntheses 8,000 h/a Operating time electrolyzer 3,000 h/a
Cost of raw materials and supplies	Electricity: 2 ct/kWh Pure water: 2,6 €/t (additionally seawater desalination)
Revenues	Electricity: no sale District heating: no sale Oxygen: no sale
Transport	up to terminal 100 km (ship, pipeline) Bundling of 10 plants to D from Morocco: 3000 km (ship or pipeline) from Middle East: 5000 km (pipeline) 12,500 km (ship) Distribution 500 km (truck, distribution network)

In the scenario for the MENA region (Middle East and North Africa, Table 33), a relatively favorable electricity price of 2 ct/kWh was assumed [135], [136], [137]. This assumes that there is still some learning curve, although there are already isolated bids below 2 ct/kWh for PV systems in the region [138], [139]. In the cost of pure water required for electrolysis, 0.6 €/t was added for the effort in desalination [140]. In the MENA scenario, in addition to the use of a CO2 point source, the case of CO2 capture from air was also considered because, depending on the location of the PtL plant, the nearest CO2 point source could be too far away for economic use. The available biomass is not considered sufficient for use for BtL processes. The transport distance cannot be estimated uniformly due to the size of the MENA region. The distance to be covered was determined for two possible cases (Morocco, Middle East) each land-based (pipeline) and for ship transport.

6.2.5. Transport costs

Against the background of the relatively large expense of a hydrogen transport [141], [142] and plans to import hydrogen from the MENA region [143], the transport costs for hydrogen and in comparison for the transport of liquid products were modeled. The approach and boundary conditions were the same as those described in Sections 6.2.1 through 6.2.4. The necessary capital costs and operating parameters were taken from the literature [141], [143] and are listed in Appendix 7. The transportation options considered in the model are:

- Truck - liquid hydrogen
- Truck - liquid fuel
- Ship (incl. import and export terminal) - liquid hydrogen
- ship (incl. import and export terminal) - liquid fuel
- Pipeline - gaseous hydrogen
- Distribution network - gaseous hydrogen

Figure 53 shows schematically the two models for transporting hydrogen. The first route (Figure 53 above) is transport by truck and, if the distance is not too short and geographical conditions permit, by ship. For this, the hydrogen is first liquefied and then transported to a terminal, which holds the hydrogen for loading onto a ship for 10 PtL plants. At the import port, there is also a terminal from which the liquid hydrogen is transported by truck to the individual consumers (e.g., hydrogen filling stations). The same approach is used in the case of a liquid product. Alternatively, the transport of hydrogen by pipeline was considered. In this case, the hydrogen also produced by 10 PtL plants is transported in gaseous form. To maintain the pressure in the pipeline, compressor stations are provided at intervals of 150 km to compensate for the pressure loss. At the end of the pipeline, the hydrogen is transferred to the consumers via a distribution network.

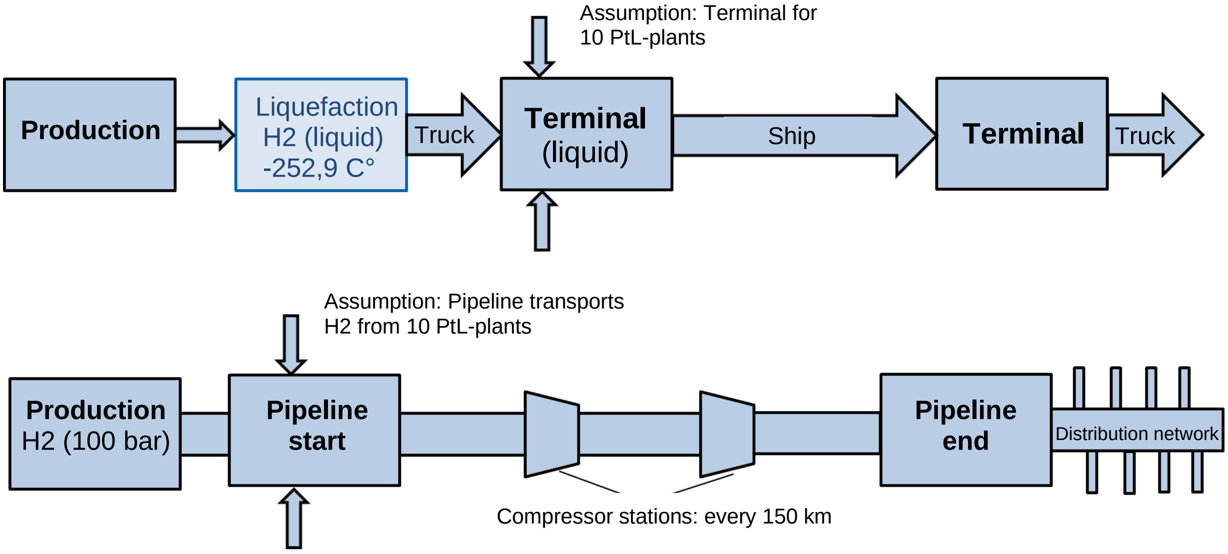


Figure 53 Transport modeling scheme (pipeline/ship and distribution)

6.3. Overview of the modeled process chains - Modular structure

For this study, process chains that serve the production of synthetic fuels were modeled. Figure 54 shows the most important steps in the production of synthetic fuels; these also correspond to individual modules, which are described in detail in the technical appendix (Appendix 5).

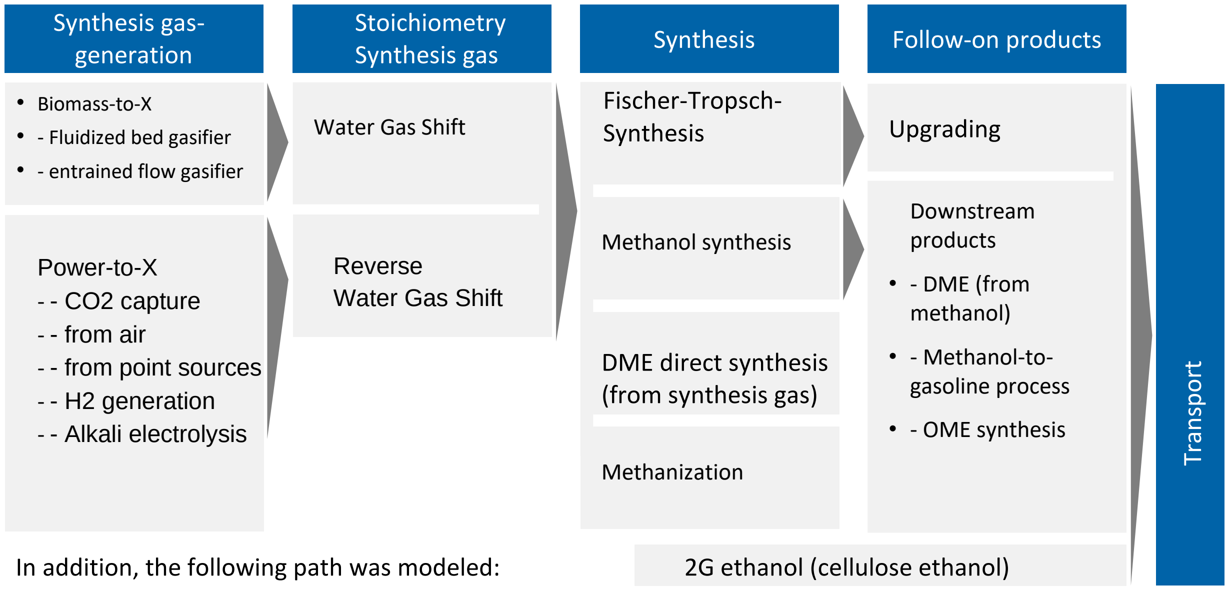


Figure 54 Modeled paths and modular structure

In addition to the production of synthetic fuels, the production of cellulosic ethanol, also referred to as "second generation ethanol," was also included in the calculations. Table 34 lists all modeled process modules, whose interconnection is shown in Figure 54.

Table 34 Overview - modeled process modules

Module	Input	Output	Type	Sources
Electrolysis	Pure water, *e*-electricity	Hydrogen, oxygen	Material/energy flows from literature data	[144] [8] [10] [128] [145] [146] [143] [98] [147]
CO2 capture from air (DAC - direct air capture)	Air	Carbon dioxide (concentrated)	Material/energy flows from literature data	[75] [8] [148]
CO2 capture from point source	Gas with increased CO2 content (e.g.: flue gas, biogas)	Carbon dioxide (concentrated)	As CO2 price	[130] [85] [148]
Fluidized bed gasifier	Biomass	Synthesis gas (hydrogen, carbon monoxide)	Aspen Plus model	[123] [149] [150] [151] [124] [152]
entrained flow gasifier	Biomass	Synthesis gas (hydrogen, carbon monoxide)	Aspen Plus model	[153] [154] [151] [150] [149] [152] [124]
Cellulose ethanol	Lignocellulose (straw, wood)	Ethanol	Model in Excel	[65] [155] [156] [157] [66] [67] [158] [159] [160]
Water Gas Shift	Water, carbon monoxide	Carbon dioxide (concentrated)	Aspen Plus model	[128] [161] [162]
Reverse Water Gas Shift	Hydrogen, carbon dioxide	Water, carbon monoxide	Aspen Plus model	[163] [164] [165]
Fischer-Tropsch-Synthesis	Synthesis gas (hydrogen, carbon monoxide	*n*-paraffin mixture with broad C-number distribution	Aspen Plus model	[166] [167] [168] [149]
Methanol synthesis	Synthesis gas (hydrogen, carbon monoxide)	Methanol	Aspen Plus model	[167] [123] [90] [169] [170] [134] [171] [172]
DME synthesis from synthesis gas	Synthesis gas (hydrogen, carbon monoxide)	Dimethyl ether	Aspen Plus model	[173] [166]
Methanation from CO2 and H2	Synthesis gas (hydrogen, carbon dioxide)	Methane	Aspen Plus model	[174] [175]
Methanation from CO2 and H2	Synthesis gas (hydrogen, carbon mnoxide)	Methane	Aspen Plus model	[176] [177] [178]

Module	Input	Output	Type	Sources
Upgrading von Fischer-Tropsch-Products (Hydrocracking)	*n*-Kerosene mixture with broad C-number distribution	Kerosene mixture of n- and iso-paraffins especially in the desired boiling range	Aspen Plus model	[179] [180]
DME synthesis from methanol	Methanol	Dimethyl ether	Aspen Plus model	[181] [182]
MtG gasoline synthesis	Methanol	MtG gasoline	Material flows from literature data, energy flows from model in Aspen Plus.	[123] [183] [169] [95] [133]
OME synthesis:				[184] [129]
Formaldehyde synthesis	Methanol	Formaldehyde	Aspen Plus model	[185] [186]
Methyl synthesis	Methanol, formaldehyde	Methylal	Material/energy flows from literature data	[187]
Trioxane synthesis	Formaldehyde	Trioxane	Aspen Plus model	[188] [189]
actual OME synthesis	Trioxane, Methylal	oxymethylene ether	Aspen Plus model	[190] [191]

Figures 55 to 57 show examples of three important process chains divided into individual process steps. These were each modeled separately and connected as modules to form the overall model. In the first two process chains, synthetic fuels are produced via the intermediate product synthesis gas. The third path shows the process scheme to produce ethanol from cellulose (2G ethanol).

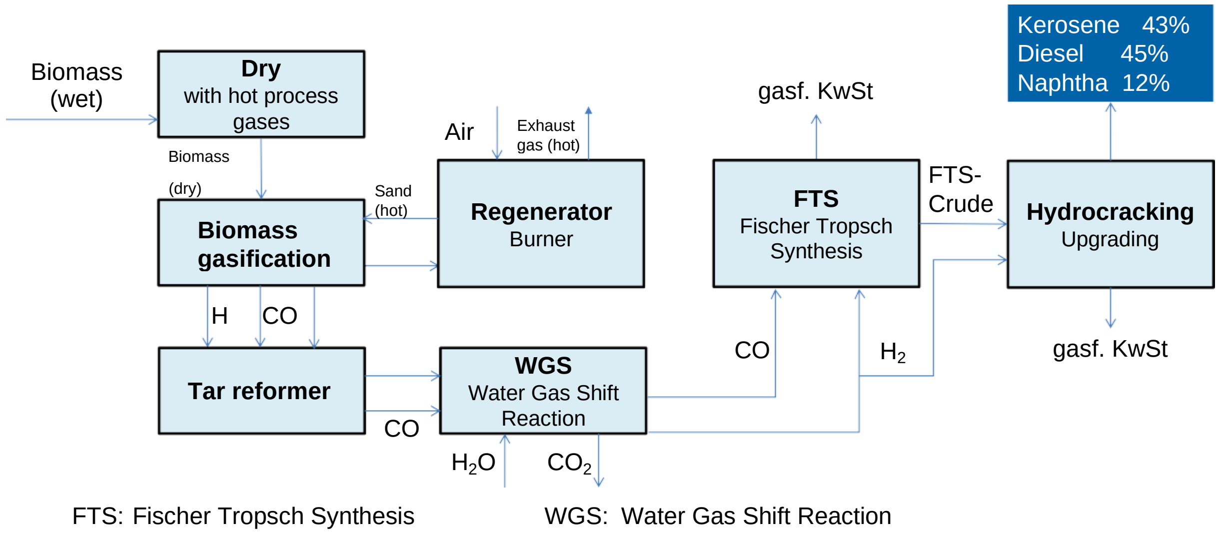


Figure 55 Modulated subprocesses - e.g. BtL fluidized bed gasification and FT synthesis

The pathway shown in Fig. 55 is based on biomass and leads via the Fischer-Tropsch synthesis to the desired products. In the example, importance was attached to a maximum yield of middle distillates. After drying and comminution of the biomass (lignocellulose, e.g. straw, wood), the actual gasification step follows within a fluidized bed of biomass and hot sand. The sand serves as a heat carrier through which the necessary energy for gasification is introduced. As a by-product, carbon is formed, which I deposited on the sand particles. This is burned in the regenerator, whereby the sand is heated up again. Another by-product of gasification is tar, which is reformed to CO and H2 with the water vapor contained in the raw gas. Before the synthesis gas can be fed to the Fischer-Tropsch reactor, the hydrogen content must be increased to the level required for synthesis (water gas shift reaction).

The synthesis yields a mixture of mainly unbranched alkanes with very different chain lengths. In order to obtain products in the desired boiling point and to improve the fuel properties, an upgrading step follows. In the example process, most of the higher molecular weight waxes produced are hydrocracked into shorter-chain middle distillates. In parallel, an isomerization of the unbranched hydrocarbons to branched hydrocarbons takes place, which leads to an improvement of the cold properties of the products. As a by-product, a certain percentage of hydrocarbons is still produced in the naphtha boiling range.

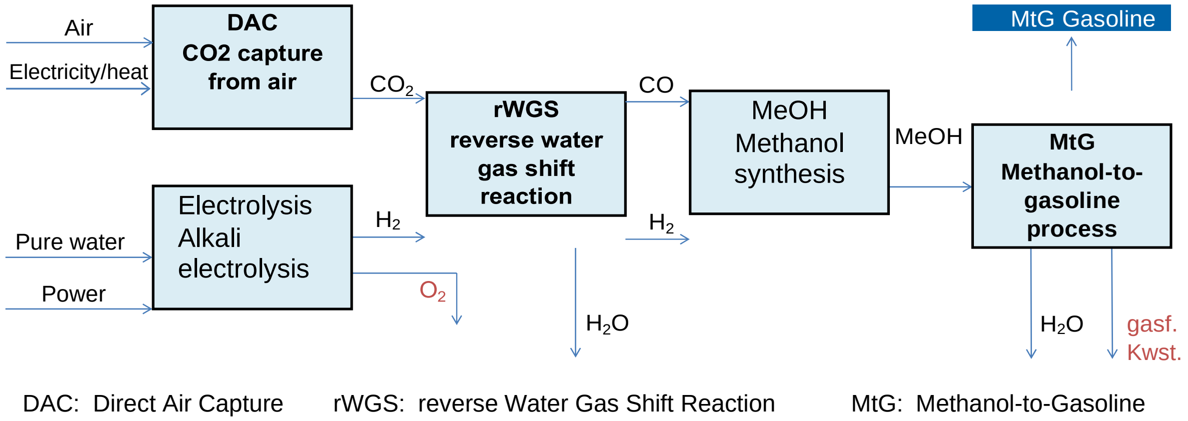


Figure 56 Modeled subprocesses - e.g. PtL methanol synthesis -> gasoline (MtG)

Figure 56 shows the synthesis of gasoline via the MtG process. The synthesis gas here comes from hydrogen produced with renewable electricity and carbon dioxide separated from the air. The hydrogen is produced via electrolysis, with oxygen produced as a byproduct. Together with the carbon dioxide separated from the air by special equipment, a synthesis gas suitable for the subsequent syntheses is produced from carbon monoxide and hydrogen via the reverse water gas shift reaction. The synthesis gas is converted to methanol using the common methanol synthesis process. In the MtG process, a gasoline-like hydrocarbon mixture is produced from the methanol. As a by-product, larger quantities of gaseous hydrocarbons are produced.

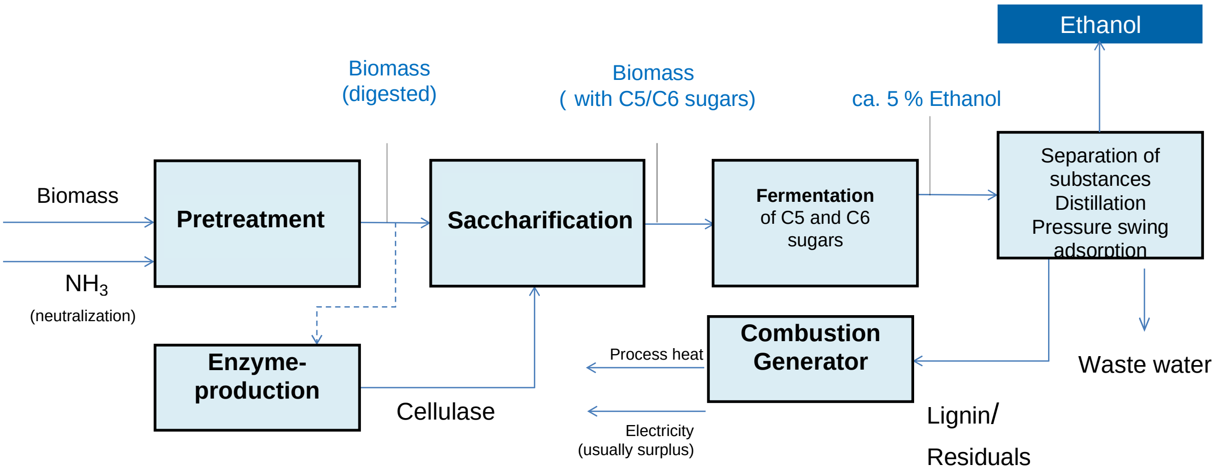


Figure 57 Modeled subprocesses - example cellulosic ethanol (2G ethanol)

In addition to the generation of synthetic products, the production of ethanol from cellulose was also modeled (Figure 57). The process control is based on the demonstration plant operated by Clariant in Straubing [67]. The shredded biomass is first soaked with hot water under pressure and digested. This increases the surface of attack for the cellulose-splitting enzymes. During this process, acidic components are released, which must be neutralized by means of ammonia. After digestion, the cellulose is broken down into sugars by certain enzymes known as cellulases. These enzymes are obtained in the same plant by means of a selective fermentation of a small partial stream of the digested biomass. The sugars are then fermented into ethanol by special yeasts that can metabolize C5 sugars in addition to the typical C6 sugars. The hemicellulose contained in lignocelluloses is composed of both C6 and C5 sugars. The ethanol, which is initially present in proportions of about 5% by volume, is then concentrated in several distillation steps. The last residual amounts of water are removed by adsorption processes to obtain anhydrous ethanol. The lignin, which cannot be converted to ethanol, and other residual materials are thermally utilized; part of the heat can be used to generate electricity.

Modeling results

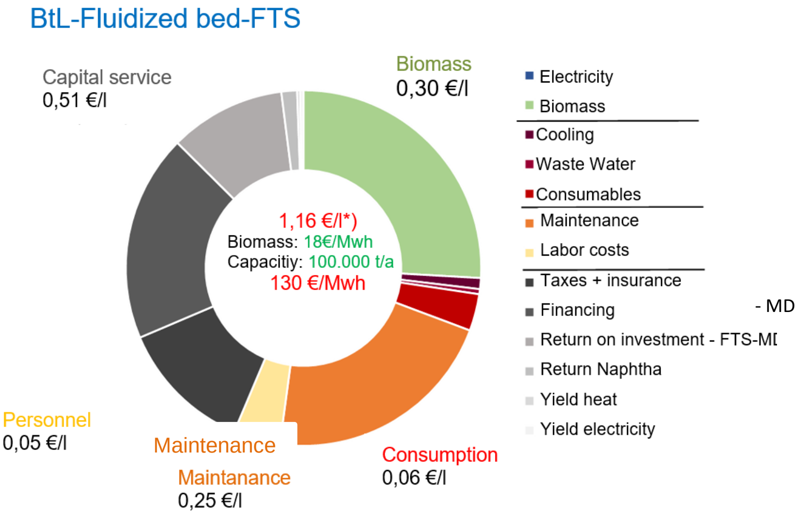
Based on the basic assumptions made in section 6.2 and considered realistic in the medium term, important parameters such as yields of products and by-products, energy, and volume flows and, from these, the costs for the economic operation of the corresponding production plant were determined for the individual paths (cf. section 6.2.4). Sensitivity analyses were carried out to assess the influence of the various parameters. For the scenarios presented in chapter 6.2.4 - Germany, Norway, and MENA - the costs for several important pathways including the transport demand were determined. At the same time, the modeling provides information on the GHG emissions associated with manufacturing and transportation.

The results allow a comparative view for the different products or manufacturing routes and production locations. Since some of the products have quite different energy densities, all data were based on liters of gasoline equivalent (LFE) for better comparability. By definition, 1 liter of petrol equivalent corresponds to the energy quantity (calorific value) of 32 MJ (equivalent to 8.88 kWh).

7.1 Product costs for synthetic products - Fischer-Tropsch synthesis

7.1.1. BtL - Biomass gasification

The synthesis gas required for the syntheses can be produced both from biomass (BtL) and from - preferably renewable - electricity (PtL). For a biomass pathway (fluidized bed/Fischer-Tropsch synthesis), the production costs (excluding transport) for the BtL product are 1.16 €/l BÄ (Fig. 58), based on the assumptions selected here for plant size (100 kt/a) and biomass price (18 €/MWh, corresponding to approx. 88 €/t DM).



*) Liters gasoline equivalent = 32 MJ = 8,88 kWh
additional assumptions: Sale of electricity: €50/MWh, heat: 20 € MWh

Figure 58 Production costs and price components BtL-FT products (biomass price 18 €/MWh, plant capacity 100,000 t/a BÄ).

The size of a plant is an important parameter influencing the economic efficiency of the process. While, as expected, the specific product costs for the required biomass are hardly influenced by the size of the plant, smaller plants have significantly higher specific costs for other price components. This applies to capital and maintenance costs as well as personnel costs (Table 31). The "downscaling" of the production capacity from 100 to 10 kt/a leads in the model to an increase in production costs to 2.08 €/l BÄ.

Table 35 Price components BtL-FT products

Cost type	**BtL-FTS small**		**BtL-FTS large**	
Biomass price Capacity	18 €/MWh **10.000 t/a** *)		18 €/MWh **100.000 t/a** *)	
Biomass	14,7 %	0,31 €/l	25,9 %	0,30 €/l
Consumption	4,2 %	0,09 €/l	4,8 %	0,06 €/l
- Water/cooling	0,6 %		1,0 %	
- Waste water	0,3 %		0,5 %	
- Other	3,4 %		3,4 %	
Maintenance	22,1 %	0,46 €/l	21,4 %	0,25 €/l
Personnel	13,8 %	0,29 €/l	4,3 %	0,05 €/l
Capital Service	45,1 %	0,94 €/l	43,6 %	0,51 €/l
- Taxes & Ins.	12,6 %		12,2 %	
- Financing	19,5 %		18,8 %	
- Return on investment	13,0 %		12,6 %	
Product price	**2,08 €/l** *) **234 €/MWh**		**1,16 €/l** *) **130 €/MWh**	

*) Liters gasoline equivalent = 32 MJ = 8,88 kWh

additional assumptions: Sale of electricity: €50/MWh, heat: 20 € MWh

In a comprehensive sensitivity analysis, the influence of several parameters on the expected costs was investigated. Only one parameter was varied in each case, in both directions; the remaining parameters corresponded to the base case (red line in Figure 59). In the tornado plot in Figure 59, the varied parameters are listed on the left and sorted from top to bottom according to the size of the influence. The large influence of capital cost is also evident here. Both varying the size of the plant and directly varying the cost of capital[17] result in the largest changes in the calculated costs. Utilization (operating hours) and lifetime, which indirectly influence capital costs, are also highly significant. The biomass price also plays a major role, while other variables have a rather small influence, although even a few ct per liter can be relevant for the profitability of a plant.

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[17] Variation of the cost of capital factor, which is multiplied by the costs stored in the model. The range of 0.55 to 1.5 used in the sensitivity analysis roughly corresponds to the range found in the literature for the cost of capital [122].

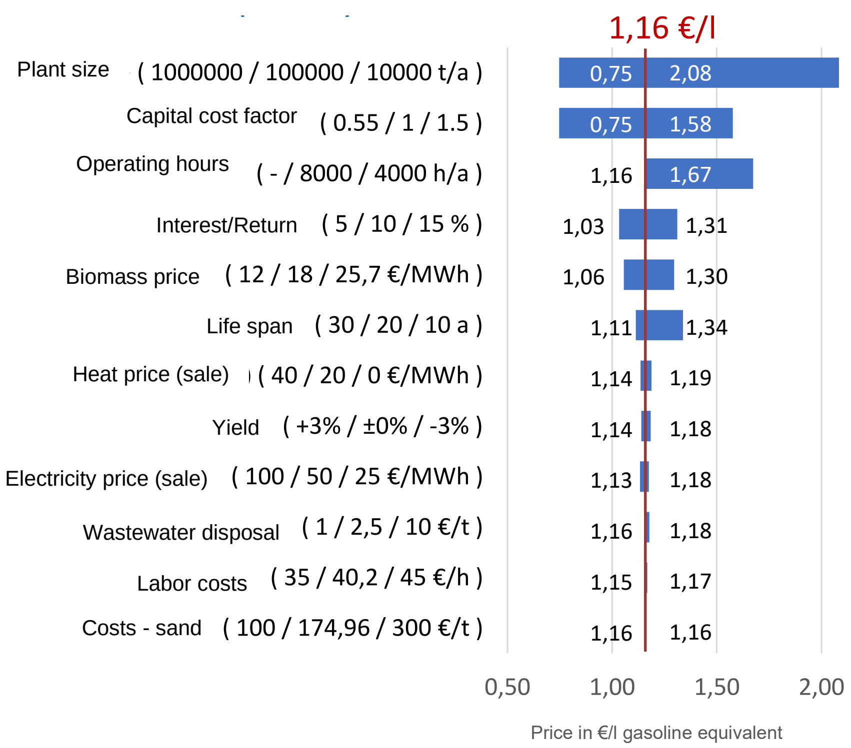
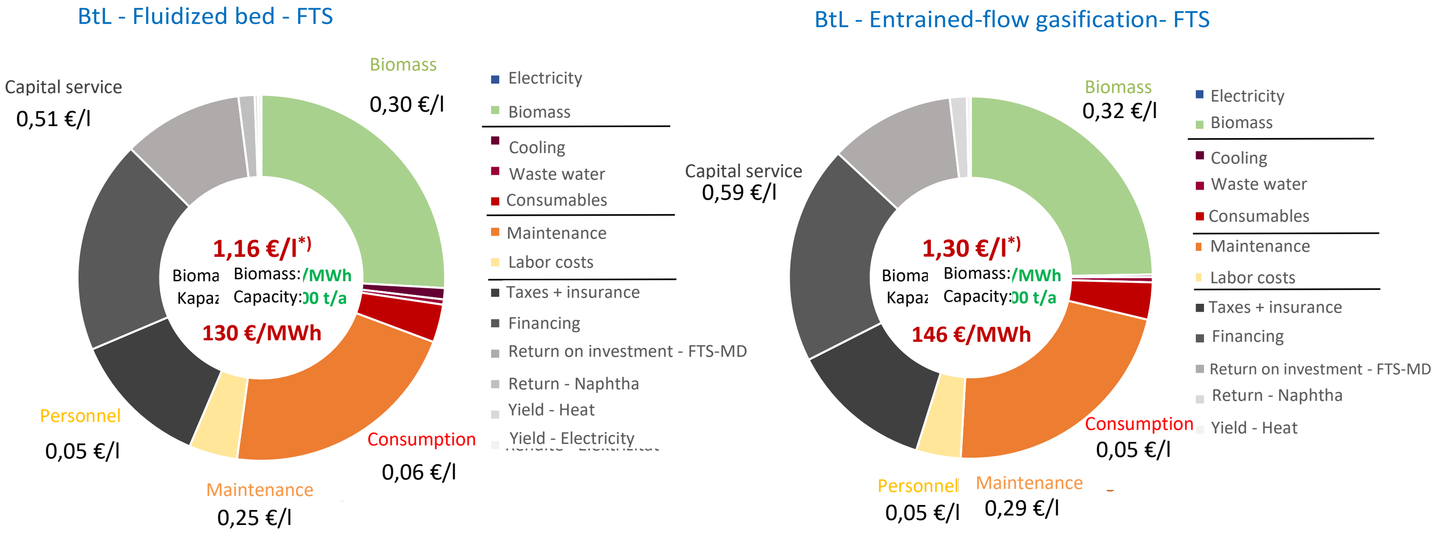


Figure 59 Sensitivity analysis BtL-FT synthesis in €/l gasoline equivalent

The second BtL route considered via entrained-flow gasification was slightly more cost-intensive in the model (Figure 60). This is due to the slightly higher assumed capital costs [152]. It should be noted that the range found in the literature far exceeds this difference [124]. The modeled fluidized bed gasification yield was also slightly higher, consistent with data from the literature [150], [192].



*) Liters gasoline equivalent = 32 MJ = 8,88kWh
Additional assumptions: Sale of electricity: €50/MWh,
heat: 20€ MWH

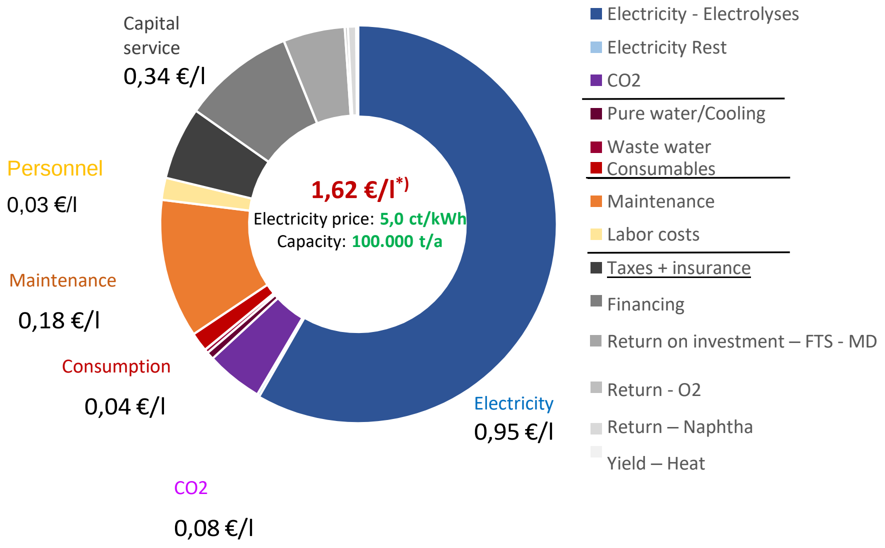
Figure 60 Comparison of production costs BtL via fluidized bed and entrained flow gasification.

However, the difference resulting with the model is small and mainly caused by the higher assumed capital costs of entrained-flow gasification. Given the fuzziness of the capital cost estimation, the difference is still within the uncertainty of the model. For BtL, only the results of fluidized bed BtL are considered in the following.

7.1.2. PtL - Electrolysis, CO2 from point source

The PtL pathway has a cost of 1.62 €/l, which is more expensive than the BtL variant in the base case. Looking at the cost structure (Figure 61, Table 36 right column), it is evident that at an electricity price of €50/MWh, this accounts for a large part of the cost of the final product. The capital costs allocated to the product costs are both absolutely and proportionally lower than in the BtL path (cf. Figure 58).

PtL: FTS



*) liter gasoline equivalent = 32 MJ = 8.88 kWh additional assumptions: Sale heat: 20 €/MWh, CO2 price (point source): 30 €/t CO2

Figure 61 Production costs and price components PtL-FT products (electricity price 50 €/MWh, plant capacity 100,000 t/a BÄ, CO2 price 30 €/t CO2).

For smaller plants of 10 kt/a bye (see table 36, left column), the costs increase, which is mainly due to the increase in capital, maintenance, and labor costs.

Table 36 Price components PtL-FT synthesis

Cost type	**PtL-FTS small**		**PtL-FTS large**	
Power price capacity	5 ct/kWh *) **10.000 t/a**		5 ct/kWh *) **100.000 t/a**	
Electricity	43,1 %	0,96 €/l	58,5 %	0,95 €/l
- - Electrolysis - - Heat - - Remainder	42,9 % 0,0 % 0,2 %		58,3 % 0,0 % 0,2 %	
CO_2	3,4 %	0,08 €/l	4,6 %	0,08 €/l
Consumption	2,7 %	0,06 €/l	2,5 %	0,04 €/l

- - Water/Cooling	0,5 %		0,6 %	
- - Waste water	0,2 %		0,3 %	
- - Other	2,1 %		1,6 %	
Maintenance	15,0 %	0,34 €/l	11,4 %	0,18 €/l

Cost type	**PtL-FTS small**		**PtL-FTS large**	
Personnel	7,6 %	0,17 €/l	1,8 %	0,03 €/l
Capital service	28,1 %	0,63 €/l	21,2 %	0,34 €/l
- - Taxes & Ins.	5,9 %		5,9 %	
- - Financing	9,2 %		9,2 %	
- - Yield	6,1 %		6,1 %	
Product price	**2,24 €/l** *) **252 €/MWh**		**1,62 €/l** *) **182 €/MWh**	

A sensitivity analysis of the PtL process shows that the electricity price has a very large leverage. At electricity costs of €20/MWh, the modeled costs are only €1.02/LCE instead of the baseline value of €1.62/LCE (red line in Figure 62) at electricity costs of €50/MWh. As with BtL processes, capital costs are another major lever. The CO2 price also plays a weighty role. More expensive processes to extract CO2 from air, at - favorably estimated - about 300 €/t CO2 [8], [79], lead to significant additional costs. Further modeling results are given in the following chapter 7.1.3. The operating hours of the electrolyzer are also of great importance for the costs. Since many of the low-cost renewable energy sources are not available around the clock, it can be strongly assumed that in many cases full-load operation of the electrolyzer cannot be achieved. The efficiency of the electrolysis is also relatively crucial, and there are currently major efforts to improve this.

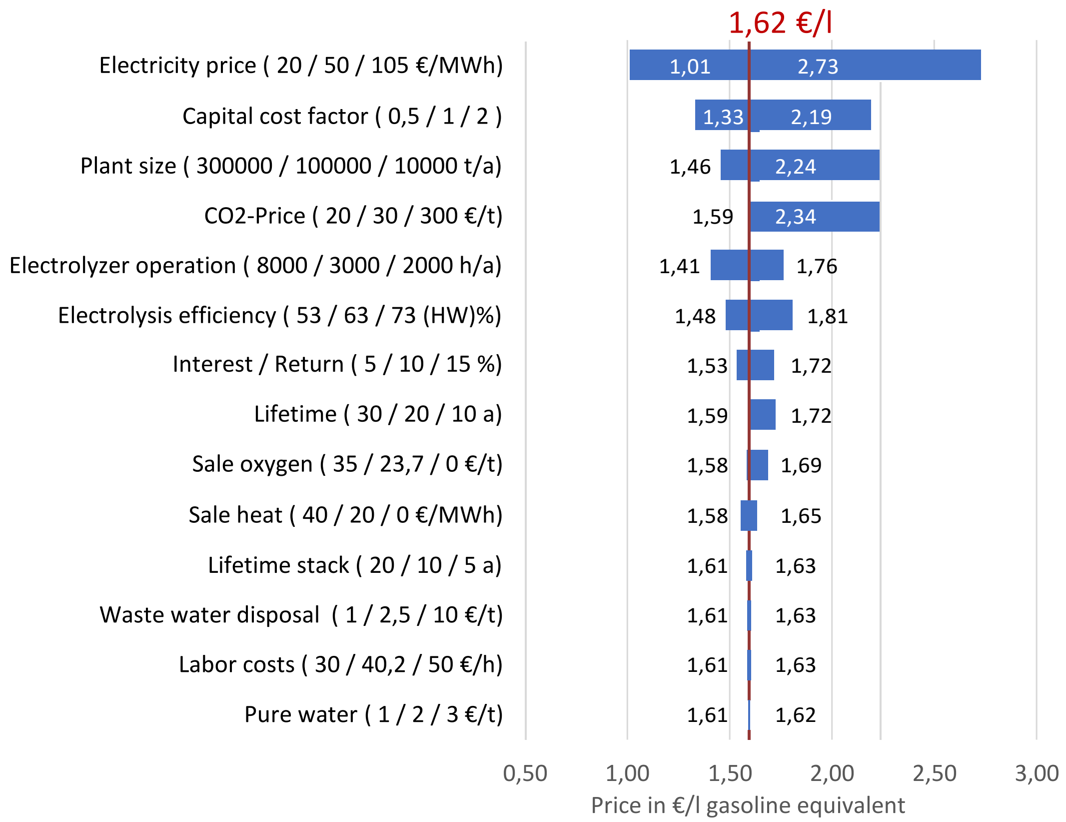


Figure 62 Sensitivity analysis PtL-FT synthesis

7.1.3. PtL - Electrolysis, CO2 from air

In the previous chapter, PtL processes with an existing CO2 point source were considered, but a CO2 point source may not always be available in remote areas. In such locations, CO2 capture from air (DAC) may be the only option for generating liquid products. While CO2 point sources were only included in the model through price, DAC was modeled directly. Therefore, CO2 costs are not shown separately in Figure 63. DAC expenses are included in the individual line items (e.g., capital costs, electricity costs, etc.).

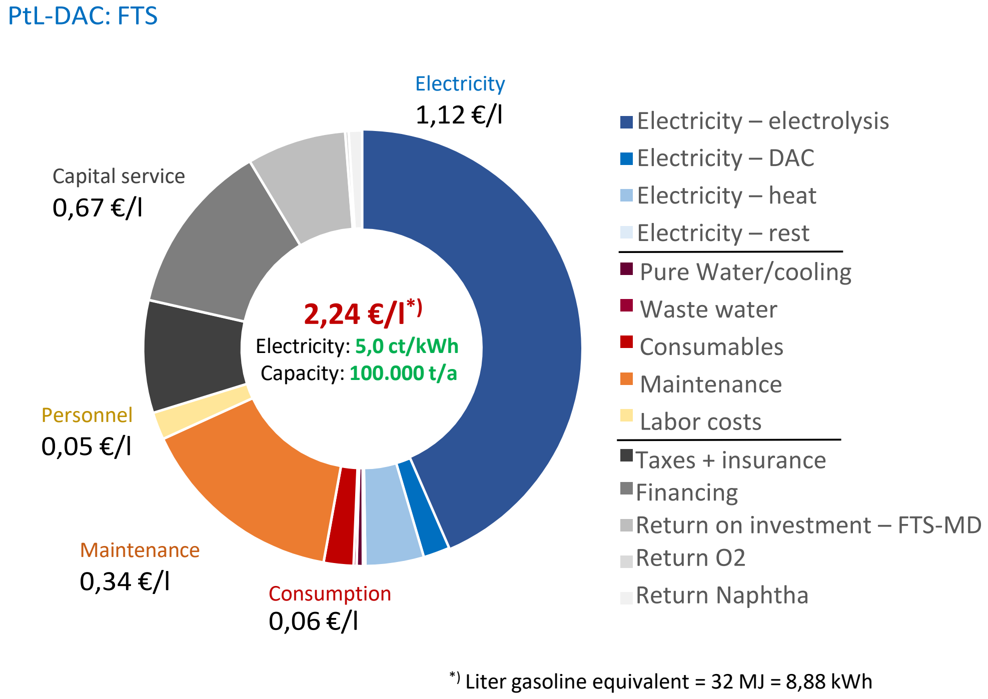


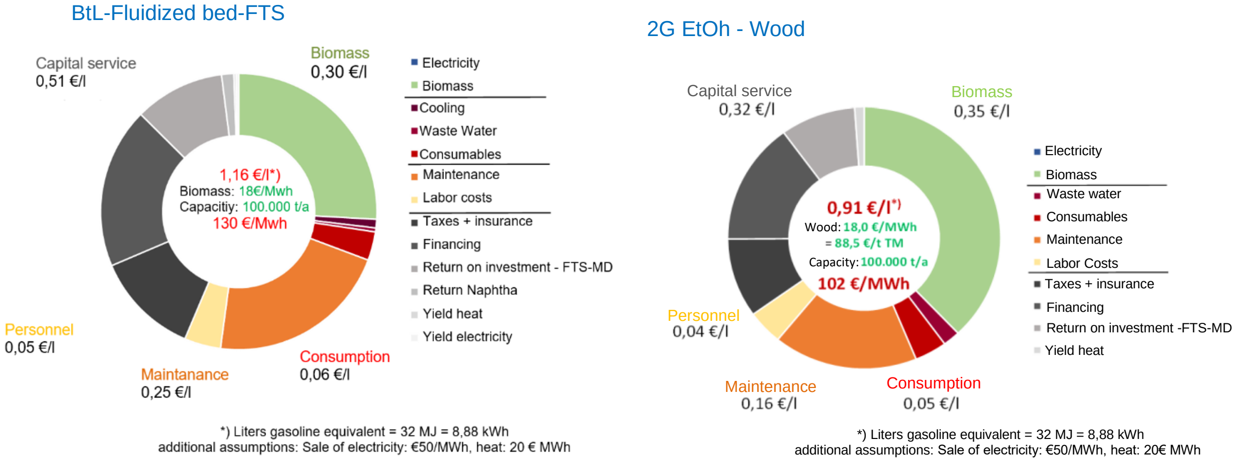
Figure 63 Production costs and price components of PtL-FT products with DAC (electricity price 50 €/MWh, plant capacity 100,000 t/a BÄ)

If the additional costs incurred for DAC in the standard case are determined in the model, this results in a CO2 price of 277 €/t CO2. This means that the costs for DAC are about a factor of 10 higher than for the use of CO2 point sources.

7.1.4. Comparison with cellulosic ethanol

In the near future, cellulosic ethanol will also play an important role as an advanced fuel alongside synthetic fuels.

BtL processes are somewhat more cost-intensive in the model than processes for cellulosic ethanol production (Figure 64). The main reason is the higher capital costs for the BtL processes, which are mainly incurred for biomass gasification and Fischer-Tropsch synthesis. As can also be seen in Figure 64 from the higher costs for cellulosic ethanol for the same type of biomass, the energy yield is higher for BtL processes. In contrast to cellulosic ethanol production, BtL also utilizes the lignin contained in the biomass as a material. However, this cannot compensate for the higher capital costs.



*) Liters gasoline equivalent = 32 MJ = 8,88 kWh
additional assumptions: Sale of electricity: €50/MWh, heat: 20 € MWh

*) Liters gasoline equivalent = 32 MJ = 8,88 kWh
additional assumptions: Sale of electricity: €50/MWh, heat: 20€ MWh

Figure 64 Comparison of production costs for 2G ethanol and BtL-FT synthesis

Cellulosic ethanol extraction for wheat or corn straw results in costs of 0.84 €/l BÄ and 0.75 €/l BÄ, respectively (Table 37). The slightly lower prices compared to "wood ethanol" (0.91 €/l BÄ) are due to the more favorable raw material prices assumed; at the same raw material price, extraction from wood would be cheapest in the model.

Table 37 Price components cellulosic ethanol

Cellulosic ethanol feedstock:	**Wood**		**Wheat straw**		**Corn straw**	
Biomass price (energy) Biomass price (mass) Capacity	18 €/MWh 88,5 €/t TM **100.000 t/a** *)		13,6 €/MWh 63,5 €/t TM **100.000 t/a** *)		7,2 €/MWh 31,5 €/t TM **100.000 t/a** *)	
Biomass	37,9 %	0,35 €/l	34,2 %	0,29 €/l	20,3 %	0,15 €/l
Consumption	5,8 %	0,05 €/l	5,8 %	0,05 €/l	8,9 %	0,07 €/l
- Waste water	2,0 %		2,1 %		2,6 %	
- Other	3,8 %		3,8 %		6,2 %	
Maintenance	17,1 %	0,16 €/l	18,3 %	0,15 €/l	21,7 %	0,16 €/l
Personnel	4,2 %	0,04 €/l	4,4 %	0,04 €/l	5,6 %	0,04 €/l
Capital Service	34,9 %	0,32 €/l	37,3 %	0,31 €/l	43,5 %	0,32 €/l
- Taxes & Ins.	9,8 %		10,5 %		12,4 %	
- Financing	15,1 %		16,1 %		19,1 %	
- Return on Investment	10,0 %		10,7 %		12,0 %	
Product price	**0,91 €/l** *) **102 €/MWh**		**0,84 €/l** *) **94 €/MWh**		**0,75 €/l** *) **84 €/MWh**	

*) liter gasoline equivalent = 32 MJ = 8.88 kWh (equivalent to 1.513 liters ethanol) additional assumptions: Sale electricity: 50 €/MWh, heat:20 € MWh

7.2 Comparative view for standard frame conditions

7.2.1. Yield

The energetic yields (efficiencies) resulting from the model are shown in Figure 65 for different BtL (fluidized bed) and PtL(with point source CO2) products. They were determined as the quotient of the heating value Hi of the product and the energy expended (heating value Hi of the biomass or amount of electricity E) (equation 28).

$$\eta = \frac{H_{i,Product}}{E} \quad \text{or} \quad \eta = \frac{H_{i,Product}}{H_{i,Biomass}} \tag{28}$$

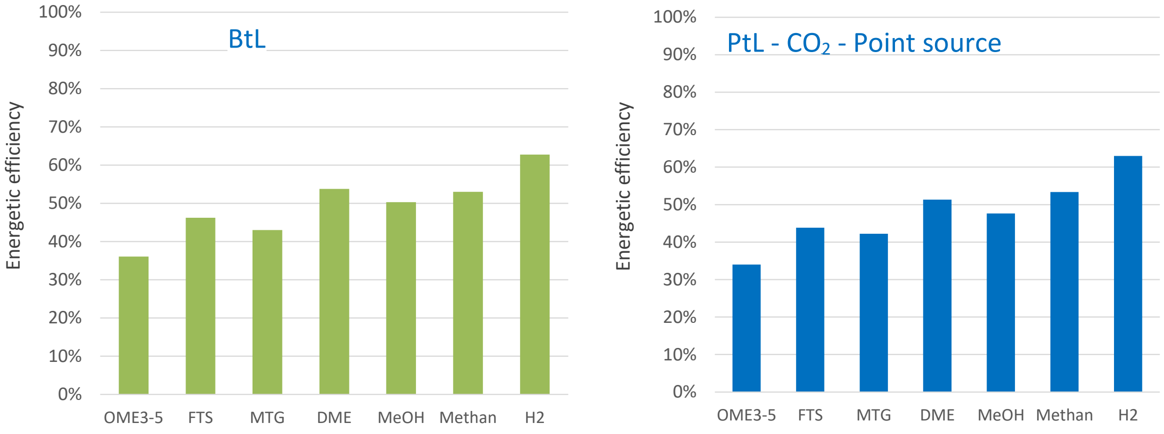


Figure 65 Comparison of efficiency of different BtL and PtL products

Yields are generally slightly higher for BtL processes than for PtL processes. Hydrogen production is an exception. The required conversion of biogenic carbon to carbon dioxide compensates for the energy advantage of BtL processes. For the products, a relatively clear ranking can be seen, hydrogen being the most favorable product. Simple molecules such as methanol (MeOH), dimethyl ether[18] (DME) and methane are comparatively easy to produce. The production of more complex product mixtures, as in methanol-to-gasoline synthesis and Fischer-Tropsch synthesis, is more energy intensive. OME synthesis is associated with the lowest yield. This is due to the release of some of the energy chemically bound in the methanol during the formation of the intermediate formaldehyde.

7.2.2. Product costs

Figure 66 shows the product costs for BtL pathways and PtL pathways with CO2 point source. Hydrogen can be produced most cheaply in comparison, followed at some distance by simple molecules (methanol, dimethyl ether, methane). The production of product mixtures (Fischer-Tropsch synthesis and methanol-to-gasoline) is somewhat more expensive. By far the most cost-intensive route is the production of OME. One reason for this is that the yield decreases with increasing complexity of production (see Fig. 65). This means that more feedstock is required. In addition, the capital costs for the synthesis plants usually rise with increasing complexity of the processing.

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[18] direct DME path from synthesis gas

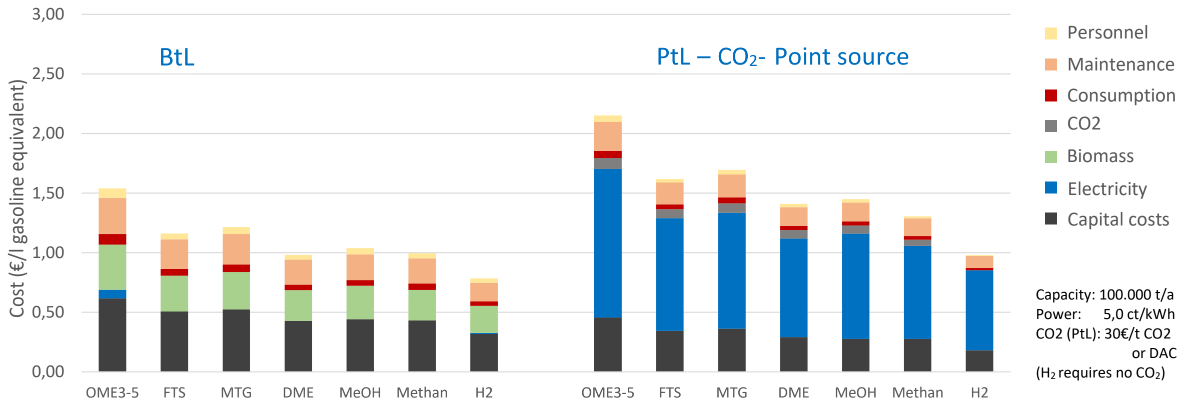


Figure 66 Cost comparison for synthetic fuels

Under the basic assumptions made in chapter 6.2 - here the plant size of 100,000 t/a BÄ, an electricity price of 50 €/MWh, and a biomass price of 18 €/MWh - the BtL processes turn out to be more cost-effective than the respective PtL processes. However, this is strongly dependent on the framework conditions, especially the electricity price plays a major role. For the Fischer-Tropsch synthesis, a price parity between the BtL and PtL processes would occur in the model at an electricity price of about €27/MWh.

If the carbon dioxide does not come from point sources, but is captured directly from the ambient air via so-called *direct air capture* (DAC), the costs increase significantly (Figure 67). The effort required to capture the CO2, which is only present in very low concentrations in the air, is many times higher than when using highly concentrated CO2 sources [193], [80].

As long as sufficient CO2 point sources are available (see Section 2.3), priority should be given to using this carbon dioxide for PtL syntheses. This does not lead to additional CO2 emissions during the use of the fuels, since the CO2 released by the emitting process would otherwise also be released into the atmosphere. Capturing the CO2 from air would therefore only be a (very costly) detour that should be avoided if possible. Due to the lower energy requirement, capture from a point source can ultimately substitute even more fossil carbon dioxide than the use of air CO2 (see also section 2.3).

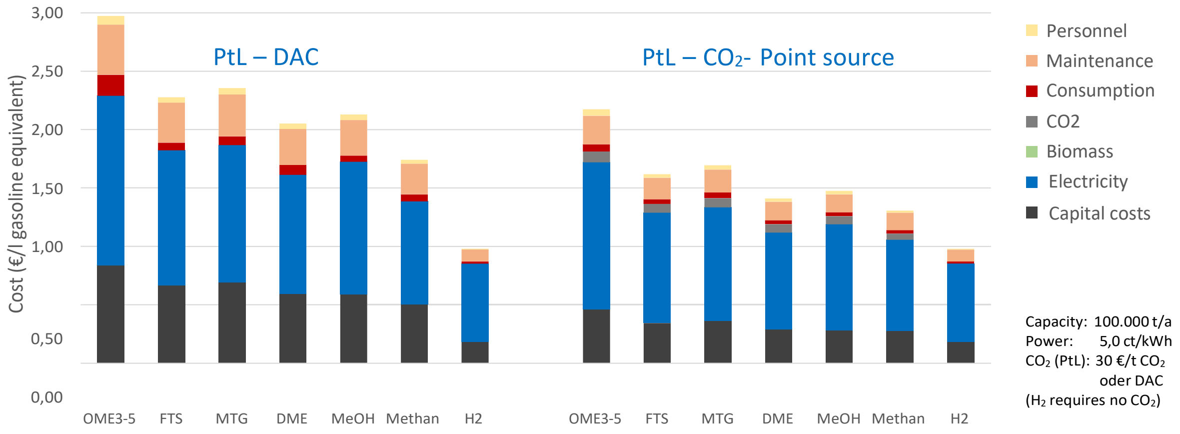


Figure 67 Cost comparison e-fuels (CO2 point sources and DAC)

7.3. Manufacturing costs at different locations

In order to compare the costs for different locations, transport costs must be taken into account in addition to the actual production costs (see chapter 6.2.5). These can become significant, as can be seen in the example of hydrogen transported from Morocco by pipeline in Figure 68. In this example case, the transport costs are higher than the costs for hydrogen production. The cost increases from 0.61 €/l gasoline equivalent (equivalent to 2.28 €/kg H2) to 1.54 €/l gasoline equivalent (5.76 €/kg H2) due to the transportation effort.

It should be noted here that these costs only apply to newly constructed H2 pipelines. There are considerations that retrofitting existing natural gas pipelines can reduce the capital cost of hydrogen transport to 25% [194]. Prices of 0.13 €/kg H2 per 1000 km are given [195]. For this favorable price, it is also assumed that the amount of hydrogen transported is about 7 times higher.

Under these general conditions (only 25% capital costs, approx. 7-fold hydrogen flows, electricity-driven compressor stations), the transport costs in the model used here drop to 0.14 €/kg H2 for 1000 km. In the example for Morocco, see Figure 68, these costs are then 0.42 €/kg H2. Converted to 1 liter of gasoline equivalent, the transportation cost for pipeline transport drops from €0.76 to only about €0.11. It should be noted, however, that this approach represents a quasi decommissioning of natural gas pipelines, which would only be feasible once certain parts of the natural gas industry have been wound up. Moreover, such large quantities of hydrogen are not yet transported in the short term. In the medium term, however - the source [194] refers to the year 2040 - the costs for hydrogen transport could fall sharply as a result of these measures.

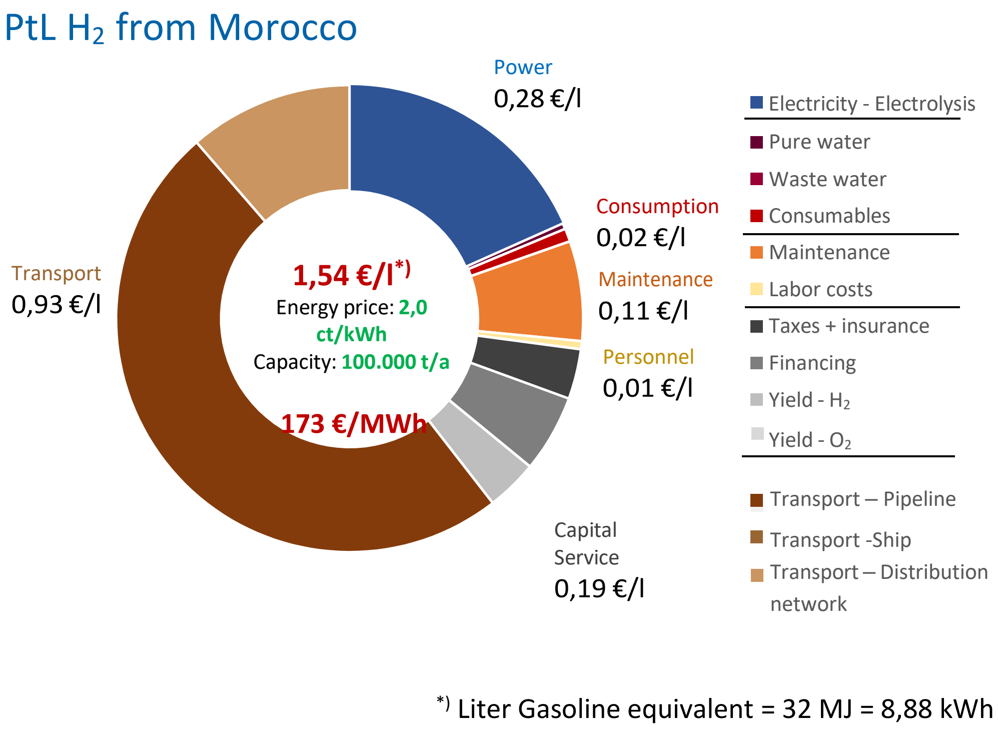


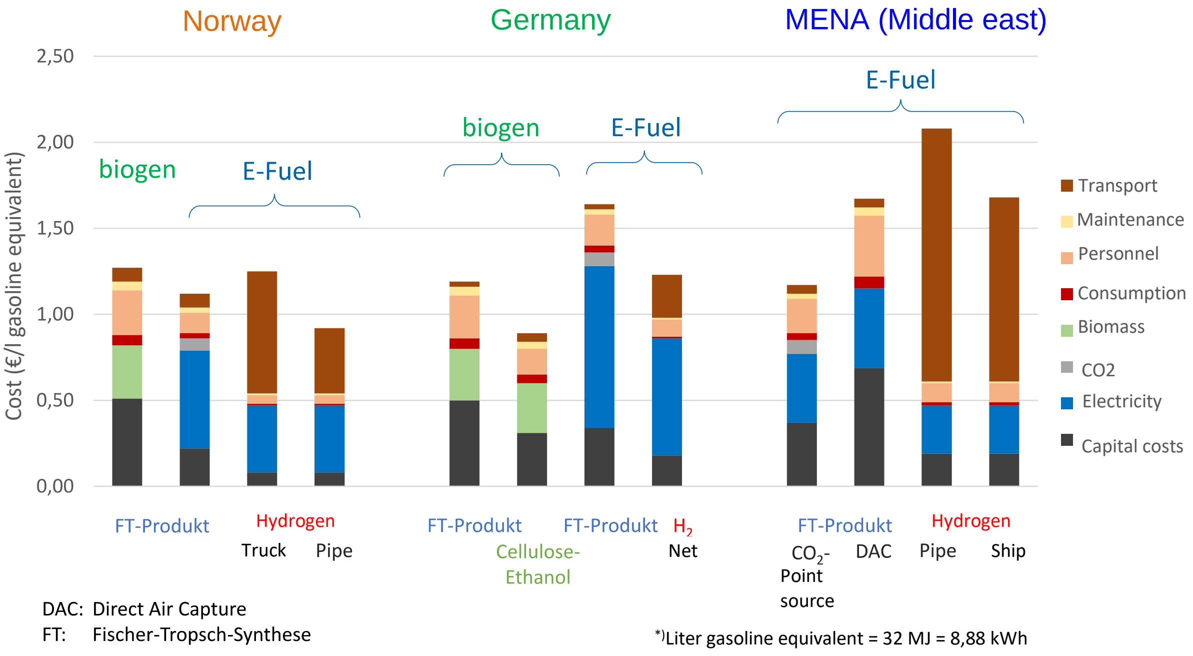
Figure 68 Product costs incl. transport (e.g. H_2 by pipeline from Morocco)

The transport costs were determined for the scenarios Germany, Norway and MENA, each for selected liquid products and hydrogen. Basically, similar basic assumptions apply to the different pathways and locations, which only differ in a few points (see section 6.2.4, tables 31 to 33). (see section 6.2.4, tables 31 to 33) and were supplemented by the transport costs.

The most important differences between the scenarios are:

- the respective assumed electricity price - Germany: 5 ct/kWh, Norway 3 ct/kWh, MENA 2 ct/kWh
- the availability of biomass and CO2 point sources - Germany and Norway have both, MENA has no biomass and only limited CO2 point sources
- the respective distance to Germany - for Norway 800 km were assumed; for the large MENA region 2 sub-regions were considered: Morocco (about 3000 km) and the Middle East (5000 km by land and 12500 by sea).

The results of this modeling are broken down in Figure 69 for some exemplary sample paths. The price range is between just under 1 €/l and 2 €/l (gasoline equivalent) for the relatively favorable conditions assumed in each of the various scenarios.



DAC: Direct Air Capture
FT: Fischer-Tropsch-Synthese

*)Liter gasoline equivalent = 32 MJ = 8,88 kWh

Figure 69 Comparison of product prices incl. transport for different locations

For the small distances in Germany, the transport costs play a rather subordinate role, the production costs dominate the price of goods. It can be seen that biomass-based processes are more economically feasible than the production of e-fuels, despite the assumption of a very favorable electricity price of 5 ct/kWh. In view of this, it is not to be expected in the medium term that very large PtX capacities will be built in Germany dedicated to fuel production. However, on a selective basis and under suitable local conditions, electricity-based processes may be useful, especially with regard to technology development and demonstration. Regardless, chemical storage of electricity in the form of hydrogen or synthetic fuels can offer an interesting option to compensate for fluctuations in electricity generation from renewable sources and to make use of the so-called surplus electricity that may occur in larger quantities.

The calculations also show that the transport costs for hydrogen far exceed those for liquid products. This largely offsets the cheaper prices for hydrogen production. Hydrogen could be produced relatively cheaply in the MENA region. However, due to the long distance to Germany and the associated transport costs, the production of synthetic products from this hydrogen for exports to Germany appears to be the more sensible route. However, unlike hydrogen, the production of liquid PtL products requires a CO2 source. If no CO2 point sources are available, which is not the case at all locations, especially in the MENA region, CO2 from air via DAC would have to be used. This would increase the cost of production to a level similar to that in Germany when using industrial CO2.

Norway has a high potential of hydropower for low-cost electricity generation. Moreover, unlike wind or solar power plants, run-of-river power plants operate largely independently of weather conditions, which means that electrolysis can be operated with significantly more full-load hours. As a result, this location offers good conditions for the generation of electricity-based PtX products, provided CO2 point sources are available. Due to the proximity to Germany, the production and transport of hydrogen could also be economical.

7.4. Interim cost summary

The supply costs calculated using the models are around 1 to 2 €/l gasoline equivalent for most synthetic products. Green hydrogen can be produced more cheaply, especially if electricity prices are very low. However, it should be used relatively close to the point of use, since the transport of hydrogen is comparatively expensive. In contrast, liquids can be transported inexpensively over long distances by sea. This must be taken into account when selecting a suitable energy carrier for importing energy to Germany. 2G ethanol, which can be obtained from lignocellulose, has the lowest production costs. The production of advanced biogenic or electricity-based energy sources is more cost-intensive than the extraction of conventional biofuels, whose possible applications are, however, limited by law, mainly for environmental policy reasons.

For the different production paths and products, the calculated production costs do not differ significantly under the same general conditions. In general, individual compounds (methanol, dimethyl ether, methane) are cheaper to produce than mixtures (Fischer-Tropsch synthesis, methanol-to-gasoline). Oxymethylene ethers (OME) have very interesting properties for some applications. However, according to the current state of the art, their production is much more complex and expensive.

From an economic point of view, the production of biogenic advanced fuels is the best option in Germany; e-fuels are comparatively expensive. The cheapest product to produce is cellulosic ethanol (2nd generation). Norway, with its renewable electricity that can be produced cheaply in run-of-river power plants, is an ideal location for the production of e-fuels, including hydrogen. The same is true for the sunny MENA countries, for which future electricity production costs of <2 ct/kWh are under discussion. However, the long distances lead to significant additional costs for the transport of hydrogen

7.5. GHG footprint

For the assessment of the GHG footprint of the pathways considered for the different production sites (cf. Figure 69), both the

- GHG backpack of the incoming material or energy flows (biomass for BtL, electricity for PtL, and other auxiliary materials such as ammonia for cellulosic ethanol) as well as

- GHG emissions that are caused by transportation

are included. Table 38 lists the specific GHG emissions of the input variables assumed for the GHG footprint modeling. Possible GHG emissions associated with the construction of the respective production plant were not taken into account.

The values given in Table 38 represent orientation values. For a specific case, the GHG intensity may deviate within certain limits. Therefore, the GHG footprint should be determined individually, as is also customary for conventional biofuels.

Table 38 Specific GHG emissions - calculation basis

Input current	specific GHG emissions	Sources
Wind Power (Germay)	6,7 g CO_2-Äq./MJ	[196]
PV (MENA)	6,7 g CO_2-Äq./MJ	[196]
Hydropower (Norway)	11,1 g CO_2-Äq./MJ	[196]
Waste wood	0,7 g CO_2-Äq./MJ	[197]
Wheat straw	1,1 g CO_2-Äq./MJ	[197]
Corn straw	5,2 g CO_2-Äq./MJ	[198]
Ammonia	2867 g CO_2-Äq./kg	[199]
Diesel (truck transport)	89,4 g CO_2-Äq./MJ	[19]
Heavy oil (ship transport)	94,5 g CO_2-Äq./MJ	[200]

Figure 70 shows the results for the example pathways together with the currently valid fossil reference value. The GHG reduction is relatively large for all pathways. The BtL pathways have slightly lower emissions here than the PtL pathways. However, renewable electricity is often assumed to be GHG-free, in which case BtL emissions would be higher.

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[19] he specific GHG emissions of diesel shown correspond to the default value according to the 38th BImSchV (94.1 g CO2 eq./MJ), which, in line with the required GHG savings quota for 2020, has been reduced by 6%.

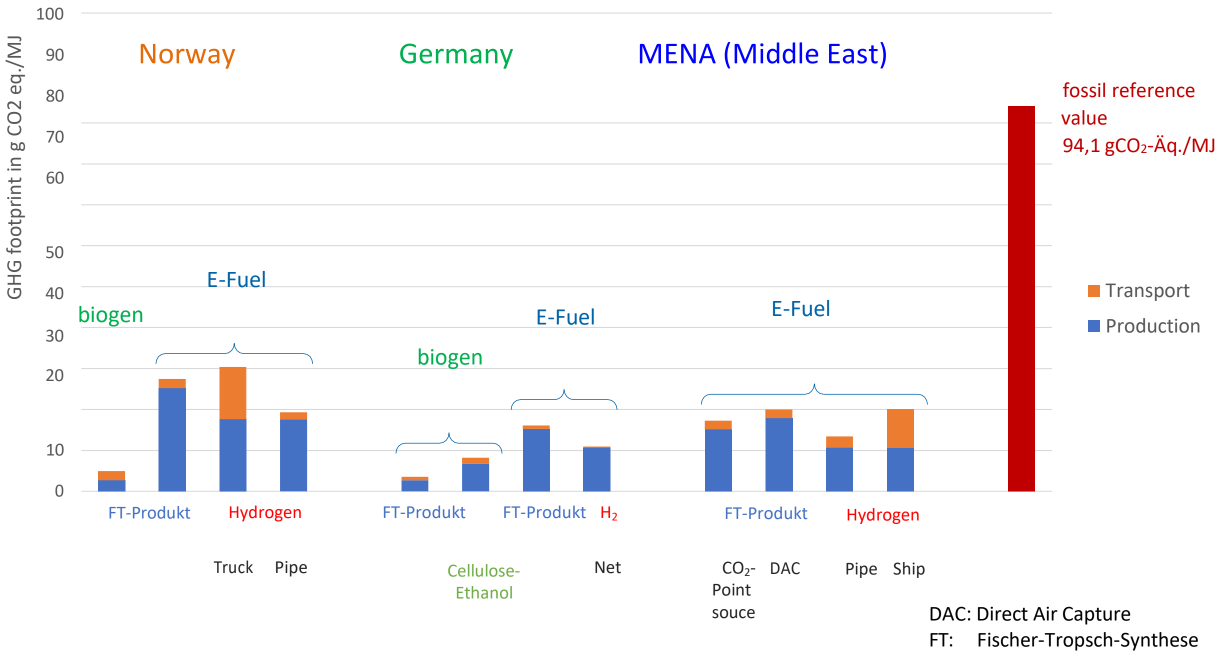


Figure 70 Comparison of GHG footprint for different production sites

Despite the use of fossil fuels, transportation only leads to comparatively low GHG emissions. Only the energy-intensive liquefaction of hydrogen for truck and ship transport has a greater impact.

7.6. Interim conclusion on GHG reduction

All advanced fuels have significant GHG reduction potential. The reduction of at least 65% compared to the fossil reference, as required by RED II, is achieved by all products considered. They can generally be considered as advanced GHG-reduced fuels.

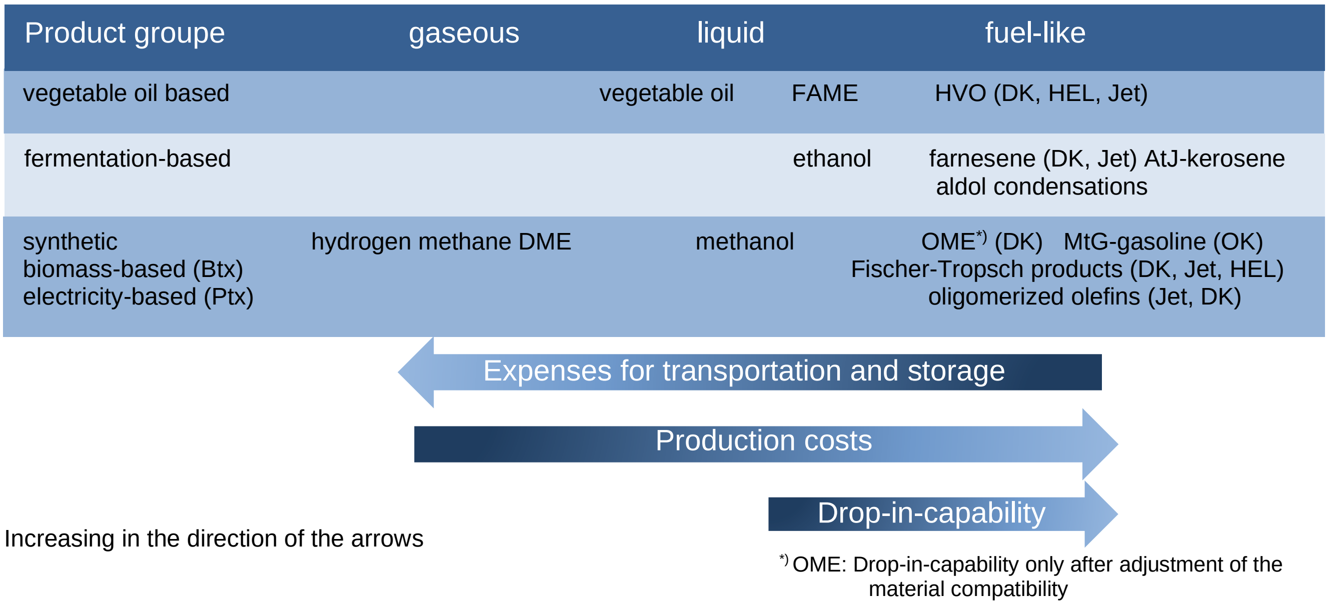
The exact GHG footprint depends mainly on the GHG intensity of the raw materials or the electricity used. The yield of the respective process also plays a role: the higher the yield, the less GHG-polluting feedstock or electricity is required.

In principle, it can be assumed that GHG emissions from advanced fuels would likewise decrease as the economy becomes more "defossilized." For example, if GHG-free alternatives to fossil diesel were used, there would be no transportation emissions from trucking.

8. Conclusion and evaluation

8.1. Summary evaluation

The success of the energy transition in transport requires the use of all possibilities to reduce greenhouse gas emissions. In addition to traffic avoidance and modal shift (road -> rail) as well as electromobility, this also includes fuels with a low GHG footprint, which can also be used to reduce emissions from conventional drives but also from heating systems (heating) towards zero (net zero emissions). Another major advantage is that at least large parts of the infrastructure (generation, transport/distribution, application) can continue to be used. A wide range of processes and products are available. "GHG-reduced" products can be divided into three groups according to Figure 71.



Product groupe	gaseous	liquid	fuel-like
vegetable oil based		vegetable oil FAME	HVO (DK, HEL, Jet)
fermentation-based		ethanol	farnesene (DK, Jet) AtJ-kerosene aldol condensations
synthetic biomass-based (Btx) electricity-based (Ptx)	hydrogen methane DME	methanol	OME*) (DK) MtG-gasoline (OK) Fischer-Tropsch products (DK, Jet, HEL) oligomerized olefins (Jet, DK)

Increasing in the direction of the arrows

*) OME: Drop-in-capability only after adjustment of the material compatibility

Figure 71 Global assessment of products and manufacturing routes

The fuel-like products generally have the best application properties for conventional applications. However, the cost of their production is usually high, resulting in high manufacturing costs. As liquid products, they are much easier to transport than gaseous substances, which is particularly important for long-distance transport (energy import). With the exception of OME, they can in principle be mixed and used in high proportions with conventional (fossil) products.

Other liquid products are also suitable as substitutes for fossil fuels. However, their chemical, physical and application properties differ significantly in some cases. They can or may therefore only be added to conventional products in certain proportions; their drop-in capability is limited.

Gaseous products (hydrogen, methane) cannot directly replace conventional liquid products. For special applications (e.g. gas engines, fuel cells ...), they also have excellent application properties. They can be produced comparatively inexpensively, but the effort and thus the costs for storage and transport are higher.

Figure 72 shows schematically and qualitatively the development of demand and efficiency in transport as well as the increasing use of alternative energy sources.

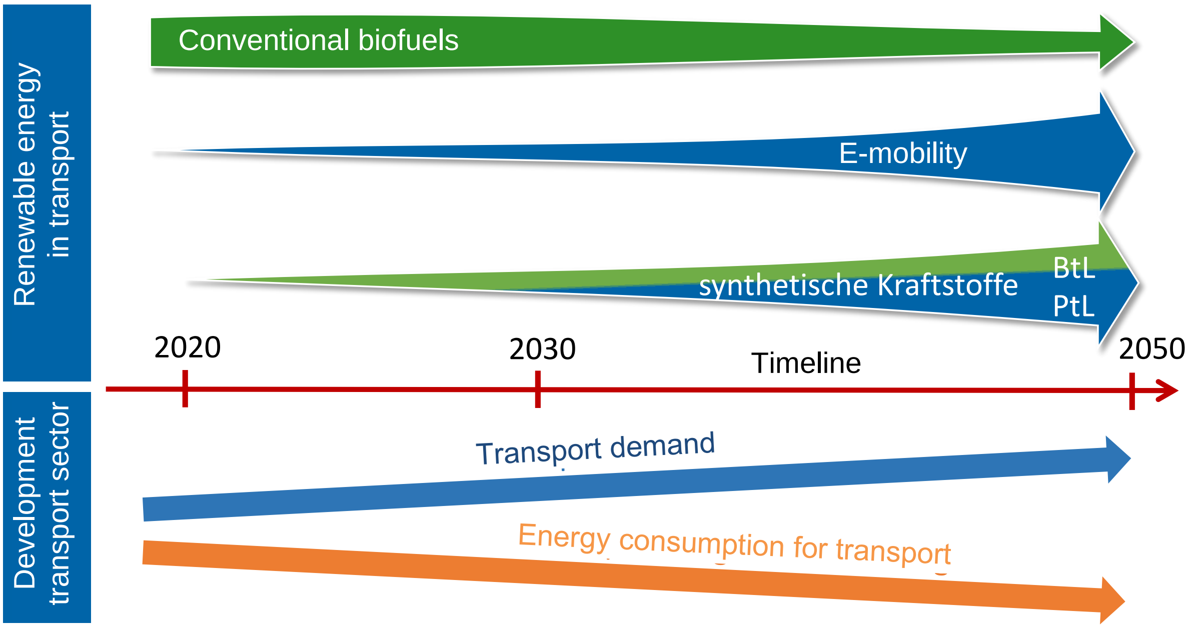


Figure 72 Developments in the transport sector

In the future, it is expected that the specific energy consumption for a defined transport performance (tonne-km, passenger-km) will continue to fall. This is due to the increasing market penetration of electric vehicles with high tank-to-wheel efficiencies, efficiency improvements for conventional drives, and a shift in traffic from road to rail. However, from today's perspective, this positive trend will be at least partially offset by a further increase in transport demand.

In order to avoid transport-related GHG emissions to a large extent, energy supply must increasingly be switched to renewable sources. In addition to
"green" electricity, advanced fuels will also make a crucial contribution to meeting energy policy goals in the transport sector. In terms of raw material availability and product quality, synthetic products have the necessary potential. From an economic point of view, the production of biogenic synthetic products or 2G ethanol is particularly interesting for Germany as a production location. In the long term, however, the biomass potential is not sufficient, so that after 2030 electricity-based products E-Fuels (PtL) will also be required. Due to the high cost of electricity in Germany, however, demand will then have to be met mainly by imports. Irrespective of this, Germany will establish itself as a driver for the development of innovative technologies and will thus also be considered as a location for corresponding demonstration objects, isolated solutions, model regions, etc. Since the technology ramp-up is not expected to the required extent in the next decade, the gradual substitution of fossil raw materials must be flanked by conventional biofuels in the short and medium term. In this context, lowering the caps for vegetable oil- or starch- and sugar-based fuels does not appear to be expedient.

8.2. Need for research

From the observations and findings of the report, a need for research in several fields can be derived.

Synthesis gas generation

Electrolysis is a key element in the generation of synthesis gas from electricity and carbon dioxide. Its efficiency can be increased at high temperatures by means of solid oxide electrolysis. However, the lifetime of electrolysers is relatively short, resulting in greater maintenance and capital costs. The reverse water-gas shift reaction required for the conversion of CO2 to CO is currently not in large-scale use; various novel process concepts are conceivable here, with which, for example, the high temperatures for the reaction can be avoided [201], [202]. At solid oxide electrolysers, syngas can also be produced by co-electrolysis of CO2 and H2O, this would save a separate reverse water gas shift reaction [203], [204], [71]. These processes are currently already in the scaling phase [205].

For biomass gasification, there is still some need for development. In principle, some pilot plants have been and are in operation. One challenge is to provide the biomass in a suitable form. The feedstock for gasification should be comparatively homogeneous. In order to achieve this, pretreatment of the biomass is required, and various concepts are being tested here [206]. Linked to this is also the logistical challenge of biomass supply, here sensible concepts for reducing transport costs must be developed.

Syntheses

The general problem with the use of renewable energies is that they mostly occur in a fluctuating manner and are therefore not available continuously and evenly. This problem can be solved by storing either the electrical energy or intermediate products - such as hydrogen - and there is potential for optimization here. Alternatively, the synthesis processes must be operated dynamically; this is also a component of current research [207].

For electricity-based fuels, syntheses from CO2 and H2 are an option; these have not yet had any large-scale significance, but could avoid a separate reverse water-gas shift reaction [207].

Optimization of the individual syntheses themselves is also important. Of the syntheses mentioned in the report, there is an increased need for research, particularly for the olefin oligomerization route of olefins produced from methanol and for OME synthesis.

Synthesis products not listed in this report could also form good power or fuel substitutes. Here, suitable substances must be identified and their application properties examined. Ammonia, for example, is currently under discussion in this regard.

Use of hydrogen

Hydrogen can be produced comparatively cheaply from renewable sources, but is limited in terms of application, storage and transport.

Hydrogen can be used in fuel cells, but these are still relatively expensive. New concepts could, for example, reduce the precious metal content or avoid it altogether. They also have certain problems with longevity. An alternative is the combustion of H2, but this causes NOX emissions that require exhaust gas aftertreatment. In the H2 denox process, on which research is currently underway, hydrogen is used directly as a reducing agent for selective catalytic reduction (SCR) of NOX. This could take place at lower temperatures (cold start) and does not require urea (AdBlue®).

Hydrogen storage, e.g. in vehicles, is either highly compressed, or in liquid form at -253°C. Here, alternative concepts such as adsorption storage could offer an advantage [208]. For larger storage and transport quantities, concepts in which the hydrogen is stored chemically in molecules (so-called liquid organic hydrogen carriers - LOHC) and can be split off again as required are also suitable [143]. Transport could also be made significantly cheaper by sharing or converting existing natural gas pipelines and networks [194].

Alternative organic oils

In order to use alternative bio-oils in a wide range, an improvement of their properties is necessary. This requires targeted upgrading steps. Due to the divergent properties of the oils, it must be examined whether established processes are suitable for this purpose and how they can be modified and adapted if necessary [103], [209]. The manufacturing process of the bio-oils could also be optimized so that the products are better suited for upgrading or even application.

Integration in refineries

As shown in section 5, many different options exist for integrating renewably produced products into refineries, of which blending of biofuels is currently in the foreground. In addition, co-processing of vegetable oils is increasingly establishing itself as a cost-effective way to produce high-quality fuels [210]. The other options presented are still at the beginning of their development. The use (production, transport, and application) of GHG-reduced H2 is currently being explored in pilot projects [211]. Primarily low-grade bio-oils could be fed together with the crude oil, for example, prior to atmospheric distillation and then processed in a targeted manner to produce products that meet standards [210]. This requires knowledge of the behavior of the individual bio-oil fractions in the subsequent refining and conversion processes. However, only a few studies are currently available on this. This also applies to the use of the entire bio-oil in various cracking processes [118].

Application

When using GHG-reduced fuels, especially if their chemistry differs from that of conventional fuels, certain problematic compounds can be increasingly produced in the exhaust gas [212], [213]. These are, for example, formaldehyde or methane, which can also be reduced with targeted exhaust gas aftertreatment concepts [214].

A large number of alternative energy sources have material compatibilities that differ from conventional fuels, which must be tested [215], [216]. Adaptations to the engine or burner control system may also be necessary. These are also necessary to fully exploit the potential of DME or OME for emission reduction, for example [213].

Increasing the allowable blending of, for example, ethanol into gasoline, or hydrogen into natural gas, which would allow greater amounts of renewables to be used without infrastructure changes, would need to be evaluated for compatibility with existing systems.

The multitude of options also creates a wide variety of blending options for fuels. Blending in new components can result in certain new effects that are not apparent when using individual components. The properties of the blended product do not always follow simple and well-known blending rules.

Economic-political framework

Various policy options need to be evaluated in terms of their suitability for promoting the use of advanced fuels. Important factors in this respect are market incentives, investment security and concepts for start-up financing.

Furthermore, the standardization process for novel feedstocks (e.g. OME) must be accompanied.

2. Summary

Model calculations were used to show that the climate targets in the transport sector, which were further tightened by the amendment to the Federal Climate Protection Act (May 2021), are unlikely to be met by electromobility alone. For the transport sector, a 48% reduction in GHG emissions compared to 1990 is required. In addition to a very ambitious electrification (10 million electric cars with 12,000 km), a shift of 10% each of passenger and freight transport from road to rail, and efficiency improvements in propulsion technology, significant amounts of alternative advanced fuels with a low carbon footprint are required to meet the climate targets in 2030 ($\approx$ 12 million tons).

Based on lignocellulose or carbon dioxide and electricity from renewable sources, high-quality, drop-in fuels can be produced to replace fossil products and close carbon cycles. The manufacturing processes offer the possibility of specifically influencing the reaction process, so that the products sometimes have better application properties than the corresponding conventional products (tailor-made fuels). As a result, the efficiency and cleanliness of internal combustion engines can be further improved. The necessary processes are known in principle and - at least in part - have already been technically tested on an industrial or demonstration scale.

Within the framework of the project, modular process models were developed with which the supply costs for advanced alternative fuels (production costs, transport costs) and the GHG emissions associated with production can be determined for variable boundary conditions using a uniform methodology. This allows comparison of different process routes and products. The determined costs fit well into the ranges known from the literature. Germany, Norway and the North Africa/Middle East (MENA) region, with their different economic and geographical conditions, were included as production locations. For these potential locations, the most favorable production paths and products could be identified:

- Germany: 2G ethanol and biogenic synthesis products,
  green H2 for hydrogenation or direct application as stand-alone solution
  Demonstration plants for E-Fuels
- Norway: E-Fuels (PtL with CO2 from point sources, H2)
- MENA: PtL (preferably with CO2 from point sources)

Regardless of open detailed questions, the main obstacle to large-scale application is the lack of viable business models or political acceptance and support.

With the final report, a generally usable calculation tool (Excel sheet) was handed over, with which the provision costs can be determined for the considered process chains under specification of variable basic conditions.

List of abbreviations

ABE	Acetone-butanol-ethanol fermentation process
aLUC	Attributive Landnutzungsänderung (engl. *attributive land use change*)
BDI	Federation of German Industry e.V.
BtL	Biomass-to-Liquid
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Usage
CFPP	Kaltfiltrierbarkeitsgrenze (engl. *cold filter plugging point*)
DAC	Direct Air Capture
DLR	German Aerospace Center
DK	Diesel fuel
DME	Dimethyl ether
E-Fuel	Electricity-based fuel
ETBE	Ethyl-*tert*-butylether
FAME	Fettsäuremethylester (Biodiesel, engl. *fatty acid methyl ester*)
FT	Fischer-Tropsch
FVV	Research Association for Internal Combustion Engines
HEFA	Hydrierte Ester und Fettsäuren (engl. h*ydrogenated esters and fatty acids*)
HEL	Heating oil extra light
HVO	hydriertes Pflanzenöl (engl. *hydrogenated vegentable oil*)
iLUC	Indirekte Landnutzungsänderung (engl. *indirect land use change*)
JRC	Joint Research Center der Europäischen Kommission
LCA	Lebenszyklusanalyse, Ökobilanz (engl. *life cycle assessment*)
LUC	Landnutzungsänderung (engl. *land use change*)
MTBE	Methyl-*tert*-butylether
MtG	Methanol-to-Gasoline
MtO	Methanol-to-Olefins Petroleum
MWV	Industry Association e.V.
OK	Gasoline
OME	Oxymethylenether
PBtL	Power and Biomass-to-Liquid
PME	Palm oil methyl ester

PtL	Power-to-Liquid
PtX	Power-to-“x-any” Products
RED	Erneuerbare Energienrichtlinie (engl. *renewable energy directive*)
RME	Rapeseed oil methyl ester
THG	Greenhouse gas (GHG)
TIC	Gesamtkosten der Installation (engl. *total installed cost*)
TPEC	Gesamtanschaffungskosten des Equipments (engl. *total purchased equipment cost*)
TPI	Gesamte Projektkosten (engl. *total project investment*)
UCO	Altspeisefette (engl. *used cooking oil*)
UCOME	Used cooking oil methyl ester
wf	anhydrous
waf	water and ash free

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Attachments

Attachments 1a	Permitted GHG annual emissions according to Climate Protection Act
Attachments 1b	Required reduction of annual GHG emissions (relative to 1990) according to Climate Protection Act
Attachments 2	Determination of final energy demand in transport
Attachments 3	Biomass potential Germany 2050
Attachments 4	Determination of specific wheel energy
Attachments 5	Process modules - technical annex
Attachments 6	Modeling of heat flows and cooling demand - technical appendix
Attachments 7	Transport - technical appendix
Attachments 8	Calculation of electricity demand for sector coupling

Attachment 1a

Permissible GHG annual emissions according to the Federal Climate Protection

Annual emission volume in million metric tons of CO2 equivalent	Basis 1990	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
Energy industry	466	280		257								175 108
Industry	284	186	182	177	172	168 165	163 157	158 149	154 140	149 132	145 125	140 118
Buildings	210	118	113	108	103 102	99 97	94 92	89 87	84 82	80 77	75 72	70 67
Transport	164	150	145	139	134	128	123	117	112	106 105	101 96	95 85
Agriculture	90	70	68	67	66	65	64 63	63 62	61	60 59	59 57	58 56
Waste management and others	38	9	9	8	8	7	7	7 6	6	6 5	5	5 4
Total	**1251**	**813**		**756**								**3011** **438**

Red values: tightening according to the amendment of the Federal Climate Protection Act of 12.05.2021 [217].

Attachment 1b

Required reduction in annual GHG emissions (relative to 1990) under the Federal Climate Protection Act.

Reduction compared to 1990 in %.	**1990**	**2020**	**2021**	**2022**	**2023**	**2024**	**2025**	**2026**	**2027**	**2028**	**2029**	**2030**
Energy industry	0	40%		45%								62% 77%
Industry	0	34%	36%	38%	39%	41% 42%	43% 45%	44% 48%	46% 51%	47% 54%	49% 56%	51% 58%
Buildings	0	44%	46%	49%	51% 51%	53% 54%	55% 56%	58% 59%	60% 61%	62% 63%	64% 66%	67% 68%
Transport	0	8%	12%	15%	18%	22%	25%	29%	32%	35% 56%	38% 41%	42% 48%
Agriculture	0	22%	24%	25%	27%	28%	29% 30%	30% 31%	32%	33% 34%	34% 37%	35% 38%
Waste management and others	0	77%	77%	79%	79%	82%	82%	82% 84%	84%	84% 87%	87%	87% 89%
Total	0	35%		40%								57% 65%

Red values: tightening according to the amendment of the Federal Climate Protection Act of 12.05.2021 [217].

Attachment 2

Determination of the final energy demand in transport

In a first step, based on a required transport performance, the energy demand is determined, broken down by energy carrier types (DK, OK, gases, electricity). In this process, the degree of electrification, the distribution among different means of transport and, if necessary, efficiency improvements can be specified or varied (different scenarios). In the second step, a fuel/energy carrier mix is quantified in detail, which also includes the required quantities of GHG-reduced fuels and/or the degree of electrification for meeting the climate targets. For this purpose, the demand for the different fuels/energy carriers is successively determined in the following order:

1. quantity of advanced biofuels (BtL diesel, cellulosic ethanol) to meet the minimum share according to the revised version of the 38th BImSchV (2.6 energy % in 2030),
2. quantity of UCOME (methyl ester of used cooking oils) as maximum chargeable share according to 38th BImSchV (1.9 energy-%),
3. quantity of conventional biofuels from food and fodder crops (FAME, ethanol) considering the calculated UCOME or cellulose ethanol quantities (upper limits according to fuel standardization: 7 vol.-% and 10 vol.-%, respectively), verification whether upper limit according to 38th BImSchV (< 4.4 energy-% from 2022) is met,
4. supplementary amount of HVO until upper limit for biofuels from food and feed crops of 4.4 energy-% according to 38th BImSchV is reached,
5. quantity of additional advanced fuels needed to meet climate targets.

The model takes into account an upper limit for paraffinic fuels (e.g. HVO and FT diesel) of 26% by volume. If the demand for advanced fuels exceeds this value, conventional gasoline is replaced by synthetic gasoline. Furthermore, the different energy contents and densities of the individual fuels are also taken into account. However, in interaction with the limitations and minimum quotas, these lead to shifts in the volume proportions whenever the energy fuel composition changes. Since this means that many variables are interdependent, the fuel composition must be determined in the model in a comparatively complex iterative process to ensure that all boundary conditions are met.

Attachment 3

Biomass potential Germany 2050 (FNR)

Estimate of domestic biomass potential in 2050 [29]

	Total potential by 2050	still unused today (in PJ)	Source
Energy from agriculture			
Energy crops*)	732	66 %	AFC, FNR, KTBL, BMERV/BMU
Straw	142	99 %	DBFZ
Liquid manure and dung	114	61 %	DBFZ
Energy from wood			
Forest and weak wood	343	64 %	DBFZ
Energy wood from the Forest (not from residues)	90	0 %	AFC, DBFZ
Landscape waste	46	33 %	DBFZ
Industrial waste wood	123	0 %	DBFZ
Waste wood	95	0 %	DBFZ
Energy from waste			
	134	3 %	DBFZ
Total	1.819	51 %	

*) Assumptions: 4 million ha arable land, yield 10 t/ha, energy content 18.3 GJ/t

Sources of the numbers:

Annex to the "National Biomass Action Plan for Germany", BMELV/BMU, 2009.

"Biomass potentials of residual and waste materials - status quo in Germany", German Biomass Research Centre DBFZ, 2015.

"Survey of statistical data on prices, cultivation and processing of renewable raw materials," AFC Consulting Group (commissioned by FNR), 2015.

"Energy consumption in Germany in 2014," AG Energiebilanzen e.V., 3/2015.

"Development of Energy Markets - Energy Reference Forecast," here: "Target Scenario," Energy Economics Institute at the University of Cologne, Gesellschaft für wirtschaftliche Strukturforschung, Prognos (commissioned by the BMWi),2014.

FNR: Cultivation of renewable raw materials in Germany, 2015 FNR: Guide to solid biofuels, 2014.

KTBL: Energy crops - data for planning energy crop cultivation, 2nd edition, 2012.
"Ecologically optimized expansion of the use of renewable energies in Germany", here: "Scenario NaturschutzPlus," BMU 2004.

Attachment 4

Determination of the specific wheel energy

As an absolute quantity, transport related GHG emissions are largely determined by energy consumption and thus by the realized transport performance. In order to clarify the influence of transport demand on the amount of advanced fuels required to meet climate targets and to demonstrate the effects of various measures, the term "wheel energy" was introduced. This refers to the amount of energy that must be available at the drive wheels to propel the vehicle. With the help of wheel energy, different transport performances (passenger- or tons-km) in road and rail transport can be linked to an energy requirement. This quantity is independent of efficiency, so that drive systems with different efficiencies can be considered. The wheel energy for the respective means of transport is the product of the specific wheel energy e_W and the corresponding transport performance (in passenger- or ton-km). The specific wheel energy e_W can be estimated according to equation (1) from the energy content E_T of the final energy carriers consumed in an area, the transport services s_T performed in the area and the associated tank-to-wheel efficiencies η_{TTW}.

$$e_W = \frac{E_T \cdot \eta_{TTW}}{s_T} \tag{1}$$

The specific load energies of the individual transport sectors are listed in Table 39. The official figures for final energy consumption and transport performance in the individual transport sectors for 2017 [218] and the tank-to-wheel efficiencies from the report [219] served as the basis for calculation; the efficiencies of buses and diesel-powered rail vehicles were equated with the efficiencies of trucks.

Table 39 Specific wheel energies and tank-to-wheel efficiencies for different modes of transportation.

Area	Specific wheel energy	Means of transport	Tank-to-Wheel-Efficiency η_{TTW}
Passenger transport (road)	0,625 PJ/billion Passenger-km	Car (OK)	28,7 %
		Car (DK)	30,5 %
		Car (elektrisch)	80 %
		Bus (DK)	42 %
Freight transport (road)	0,425 PJ/billion tons-km	Truck (DK)	42 %
Rail transport	0,183 PJ/billion Passenger- or tons-km	Rail (DK)	42 %
		Rail (electric)	85 %

Due to the higher logistical efficiency, only a fraction of the wheel energy is required for the same passenger and ton kilometers in rail transport compared to road transport. According to the Austrian Federal Environment Agency [220], a reduction in wheel energy to 37 % for rail passenger transport and 38 % for rail freight transport can be derived compared to the respective road transport. According to the same source, the required wheel energy for buses is 28 % compared to private motorized transport.

Attachment 5

Process modules - technical appendix

At this point, the technical details of the process modules presented in an overview in chapter 6.2.4 will be described in more detail. Most of the process modules were modeled in the Aspen Plus software. This modeling was partially simplified, the modeling of some auxiliary units is missing, and the processes have not been subjected to intensive optimization. Nevertheless, a good and comparable estimation of the material yields and energy flows can be assumed.

The capital costs of the individual modules have not been modeled; they were determined by values given in the literature. Deviating values were taken into account via scaling factors. In addition, a conversion of the system costs from the respective reference year given in the relevant literature to the year 2018 took place.

The following processes and sub-processes were defined as modules and modeled in Aspen Plus:

- Alkali electrolysis
- CO2 capture from air (DAC)
- CO2 capture from point source
- Biomass gasification - fluidized bed
- Biomass gasification - entrained flow
- cellulose ethanol
- Water Gas Shift
- Reverse water gas shift
- Methanation from CO2 and H2
- Methanation from CO and H2
- Fischer-Tropsch synthesis
- Upgrading of Fischer-Tropsch products
- DME synthesis from syngas
- Methanol synthesis
- DME synthesis from methanol
- MtG gasoline synthesis
- OME synthesis (4 sub models)
    - Formaldehyde synthesis
    - Methylal synthesis
    - trioxane synthesis
    - OME synthesis proper

These modules are described in detail below. For the process modeling of the entire process chains, the modules are coupled accordingly, if necessary.

Alkali electrolysis

Process

The basis of all power-to-X chains is the electrolytic splitting of water into hydrogen and oxygen. There are several processes for this electrolysis, the most established process at present is alkali electrolysis. In this process, a potassium hydroxide solution acts as the electrolyte.

According to [8], the power requirement of a modern alkali electrolysis plant for 1kg of hydrogen is currently about 51.8 kWh/kg, which corresponds to a calorific value-related efficiency of 64.3 %. According to this and also other studies [144], [8], the range of the energy input also predicted for the future is between 45.7 and 62.9 kWh/kg hydrogen. On average, a reduction from the current level of approx. 52 kWh/kg to 47 to 49 kWh/kg in the future is expected.

Operating supplies

In addition to the electricity requirement, there is also a requirement for pure water. The cells of the electrolysis system have to be replaced every 10 years, which results in approx. 25 % of the capital costs [144]. In principle, the oxygen byproduct can also be sold [128].

Currents

The most important material and energy flows are given in Table 40. The stoichiometry of water electrolysis was used as a basis.

Table 40 Overview of material and energy flows for the generation of 1 kg H2 via electrolysis

	EIN		AUS	
Material flows	H_2O (pure):	8,94 kg	H_2: O_2:	1 kg 7,94 kg
Energy flows	Electricity:	190,4 MJ		

By-products

The by-product of electrolysis is oxygen, which is needed for many processes. It makes sense to select the location of the electrolyzer so that the oxygen can be sold.

Capital costs

Table 41 provides an overview of literature data on capital costs for electrolysis; all values were converted on a TIC basis (see p. 84 in section 6.2.2) using the factors mentioned. The currency base was uniformly converted to € (2018).

The highlighted value for 2030 from [8] is used as a reference point for the modeling. It is the only value shown for very large electrolysis plants and is in the range that other sources also consider plausible in the medium to long term.

Table 41 Capital costs - literature values for alkali electrolysis (TIC reference)

Plant size MW (el.)	Cost M€ (2018)	Reference year	spec. CAPEX €/kW (el.)	Source
0,0266	0,3	2008	11130	[144]
0,266	1,2	2008	4593	[144]
2,66	5,0	2008	1895	[144]
1	1,5	2020	1486	[8]
5	3,4	2020	682	[8]
1	0,8	2030	827	[8]
5	1,9	2030	379	[8]
100	***27,5***	***2030***	***275***	[8]
1	0,5	2050	547	[8]
5	1,3	2050	251	[8]
100	16,8	2050	168	[8]
1	1,6	2017	1600	[146]
2+	1,8+	2020	900	[146]
2+	1,4+	2030	700	[146]
N/A	N/A	2019	440-1231	[143]
N/A	N/A	2030	352-747	[143]
N/A	N/A	Long term	175-615	[143]
N/A	N/A	2019 – China	175	[145]
N/A	N/A	2030 – China	101	[145]

The degression coefficient χ has been estimated to be 0.76 using the data from [8].

Comments

Since the electrolysis of water is a core technology for the use of renewable energy, there are many efforts to optimize this process. For example, electrolysis requires less electrical energy when the water is in vapor form [221]. To avoid the expense of a separate subsequent reverse water-gas shift reaction, water and carbon dioxide can also be used together in a so-called co-electrolysis and processed into synthesis gas.

CO2 Capture from air

Process

In principle, when CO2 is separated from a gas (air or flue gas), the CO2 is first selectively chemically bound in an absorber. Subsequently, a desorption process takes place by adding heat, with the exclusion of air, by which very pure CO2 can be obtained. A new cycle of absorption and desorption then begins.

A major problem in the separation of CO2 from air is that air contains only small amounts of CO2, which is why large quantities of air (approx. 1.4 million m^3 [75]) must be converted for each t of CO2. This requires a correspondingly large number of large fans, which dominate the external appearance of a DAC plant and have a high energy requirement. In the absorber, only the smallest possible pressure drop should occur due to the large air volumes passing through, in order to minimize the amount of energy required for the fans.

The desorption process requires relatively large amounts of heat. These usually exceed the considerable reaction heats that would be released during the corresponding synthesis reactions.

Operating supplies

No operating materials were modeled separately.

Currents

The required material and energy flows were determined from data provided by Climeworks (according to [75], [8]). A CO2 content of 400 ppm in the air and a separation efficiency of 90 % were assumed. For the energy demand, the average values of the ranges given in [8] were used (heat: 5.4...7.2 MJ/kg, electricity: 0.72...1.08 MJ/kg. The temperature level of the required desorption heat in this process is 95 °C.

Furthermore, a compression from ambient pressure, at which the CO2 is initially present, to 30 bar was assumed for the reverse water gas shift reaction (rWGS), which also requires electrical energy. Table 42 shows the material and energy flows for the production of 1 kg CO2.

Table 42 Overview of material and energy flows during capture of 1kg CO2 from air

	On		Off	
Material flows	Air:	1821 kg	CO_2:	1 kg
Energy flows	Heat (95 °C): Electricity:	6,3 MJ 1,16 MJ	-	

Capital costs

In the study [8], certain costs are given for different sizes of a DAC plant in € (2015) are given (table 43). From these, an exponent χ for the degression of 0.79 can be determined.

Table 43 Capital costs for plants for CO2 capture from air (TIC reference)

Plant size t/a CO2	Costs M€ (2018)	Reference year	spec. CAPEX € per t/a CO2	Source
1000	1,8	2015	1798	[8]
16000	16,5	2015	1029	[8]
160000	***98,8***	***2015***	***617***	[8]
980000	619,1	2018	632	[83]
980000	428,3	Long term	437	[83]
14150	20,2	2012	1429	[80]

The scale of the plant highlighted in Table 43 is between the size that would be required to produce 10 000 t/a and 100 000 t/a of PtL product. Accordingly, while there is little need for an uncertain extrapolation of the values from [8] to estimate the capital cost of DAC for a 100 000 t/a plant. However, the value itself is probably already the result of a relatively uncertain extrapolation. The largest DAC plant constructed by Climeworks has a capacity of only 900 t/a [75]. Keith et al. described a much larger plant [83].

Comments

The amine-based CO2 adsorption considered here requires only a moderate desorption temperature of about 95 °C, so that low-temperature heat can be used. Alternatively, processes using lime and caustic potash could be used for CO2 capture [83].

Modeling indicates the process to be relatively favorable. However, very high desorption temperatures of about 900 °C are required, which in most concepts are achieved via combustion of natural gas. The CO2 that is produced in the process is also captured. In the case of storage (CCS), this would still be relatively unproblematic. However, in the case of the use considered here to produce synthetic fuels (CCU), this would lead to a significantly increased GHG footprint of the products.

CO_2- Separation from point source

Process

The process of CO2 capture from a point source basically works similarly to CO2 capture from air. Due to the high concentration, the energy required to capture most of the carbon dioxide is much lower [148].

In combustion processes, the capture of CO2 can be optimized by using pure oxygen for combustion rather than air. This increases the carbon dioxide content in the flue gas because the high nitrogen flow introduced during combustion with air is eliminated. Usually, an air separation unit is operated for oxygen production. In PtL processes, a possible synergy effect is that water electrolysis also provides oxygen as a by-product. This could eliminate the need for the energy-intensive air separation process for combustion with oxygen.

According to model calculations, the price range for CO2 from point sources is in the range of 30 to 100 €/t CO2 [85], [130]. Capture is particularly favorable for coal-fired power plants and cement plants.

No modeling was done for this process, but only a price of 30 €/t CO2 was calculated as the default case. However, the price can also be adjusted in the model.

Biomass gasification - fluidized bed

Process

The modeling of the fluidized bed gasification process was divided into several sub steps, which are shown in an overview in Figure 73. The model consists of 4 blocks. consists of several sub steps, which are shown in an overview in.

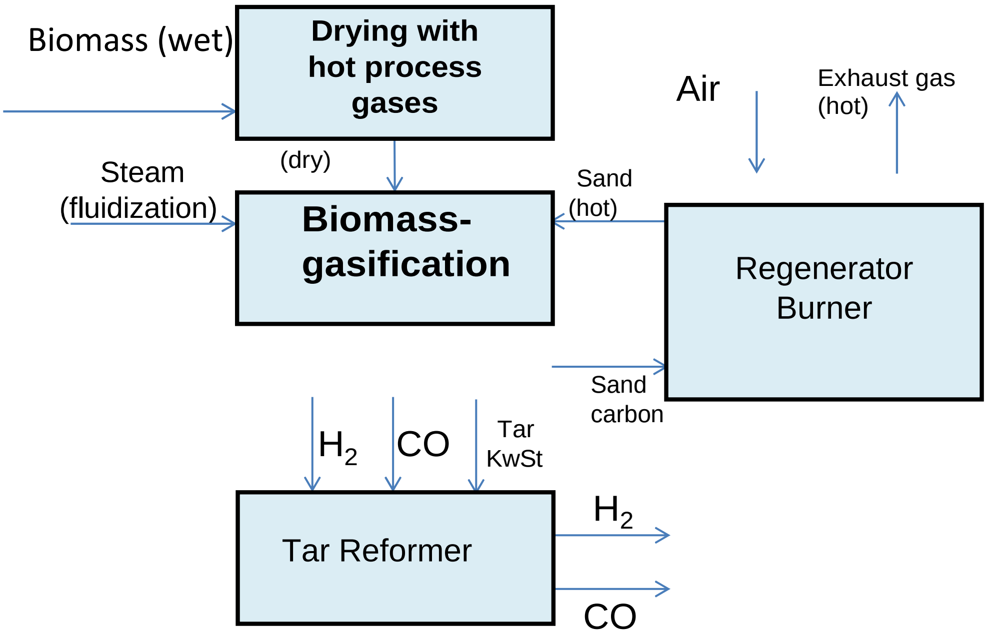


Figure 73 Process diagram biomass gasification - fluidized bed

- In the first model step, the shredded biomass is dried at 113 °C and ambient pressure. The amount of heat required for this comes from the flue gases of the regenerator. For this purpose, Aspen Plus used a stoichiometric reactor in which wet biomass (50% moisture) is converted to dry biomass (5% moisture) and water. The biomass is modeled as a non-conventional material with a composition that is typical values for poplar, a well-suited fast-growing cultivated biomass, according to data from [123].

- This is followed by the actual gasification step. This takes place in a fluidized bed, which consists largely of the heat transfer medium sand, which is used in a ratio of approx. 24:1 (sand to biomass) and supplies the necessary process heat for heating the biomass and the endothermic gasification reactions. Water vapor is used as fluidization medium for the fluidized bed. The amount here is 40% of the biomass used. The temperature is 890 °C. In the model, the fluidized bed gasifier is operated at 1.6 bar following [123]; for further syntheses, the synthesis gas must be compressed afterwards.

The gasification of the biomass is represented based on literature data [123] via a stoichiometric reactor model in which the respective conversions are specified. Coke, tar, syngas, hydrocarbons, and ash are produced.

- The coke is burned by the sand on which it is deposited in the regenerator. In the process, the sand heats up to 1125 °C, which is returned to the fluidized bed reactor. From this circuit, 0.01% of the sand is removed as purge stream and must be replaced with fresh sand. The hot flue gas is also used as a heat supplier at various points in the process.

In addition to the coke produced, a certain part (approx. 10 %) of the synthesis gas must also be burned for the heat quantities to be applied in the high-temperature range, above all for the heat supply of the tar reformer and partly also for the gasification. The combustions are modeled in a Gibbs reactor model with a λ-value of 1.2 towards the thermodynamically expected equilibrium.

- In addition to CO and H2, the resulting synthesis gas also contains methane and many higher hydrocarbons up to tar (for tar, the model component naphthalene C10H8 was used).

To remove most of these components, tar reforming is performed, in which the hydrocarbons react catalytically with the water vapor contained in the raw syngas to form CO and H2. This process is endothermic, the inlet temperature to the reactor is about 1300 °C, and the pressure is 1.6 bar, as in gasification. The cyclic regeneration of the catalyst was not considered. The turnovers of the tar reformer were taken from the literature [123] and were set as the boundary condition of a reactor model operating stoichiometrically.

Operating materials

In addition to biomass, the process requires sand as a heat transfer medium. Another operating material is the catalyst for tar reforming, which also has to be renewed continuously (3.6 % are replaced per year). According to [123], the cost of sand is 174 €/t, with 15 kg of sand required per ton of product (in the case of Fischer-Tropsch synthesis). For the renewal of the catalyst, there are only very minor annual costs of 0.016 € per t of product (in the case of Fischer-Tropsch synthesis).

Currents

Table 44 Overview of material and energy flows for the production of 32 MJ syngas (calorific value reference, equivalent to one liter of gasoline) in biomass gasification (fluidized bed)

	EIN	AUS
Material flows	Biomass*: 4,99 kg Sand: 6,74 g	CO: 1,47 kg H_2: 0,143 kg
Energy flows	Electricity: 2,78 MJ	Heat (945→230 °C): 2,72 MJ Heat (899→230 °C): 2,54 MJ Heat (113→73 °C): 0,57 MJ Heat (73→63 °C): 3,27 MJ Heat (63→40 °C): 3,20 MJ

* Water content: 50 %

Table 44 shows the most important material and heat flows, which are considered for further cost modeling. This includes a compression to 25 bar for subsequent syntheses.

Capital costs

The capital costs for the biomass gasification unit (consisting of pretreatment, gasification, and gas treatment) were obtained from various sources and tabulated in Table 45. Capital costs were selected relatively conservatively to account for uncertainties in biomass gasification implementation. In addition, a source was used that provides data for capital costs for both fluidized bed gasification and entrained flow gasification. According to [128], a degression coefficient χ of 0.755 (as the average of the reported degression coefficients of relevant parts of a biomass gasification unit) is obtained.

Table 45 Capital costs for biomass gasification in fluidized bed (TIC reference)

Plant size MW (biomass)	**Cost M€ (2018)**	**Reference Year**	**spec. CAPEX €/kW (biomass)**	**Source**
432	68,8	2007	159	[123]
389	80,8	2010	208	[149]
400	***262,3***	***2011***	***656***	[152]
300	121,6	2013	405	[172]
10	7,3	2013	731	[192]

Biomass gasification - entrained flow

Process

The schematic of entrained flow gasification is shown in Fig. 74. In contrast to the modeled fluidized bed gasification, in entrained flow gasification the required thermal energy is generated directly in the gasifier by partial oxidation. Pure oxygen is required for this, since an N2 input into the gasification would lead to dilution of the synthesis gas. The required air separation unit has an electricity demand of 0.3 kWh/kg O_2 [153].

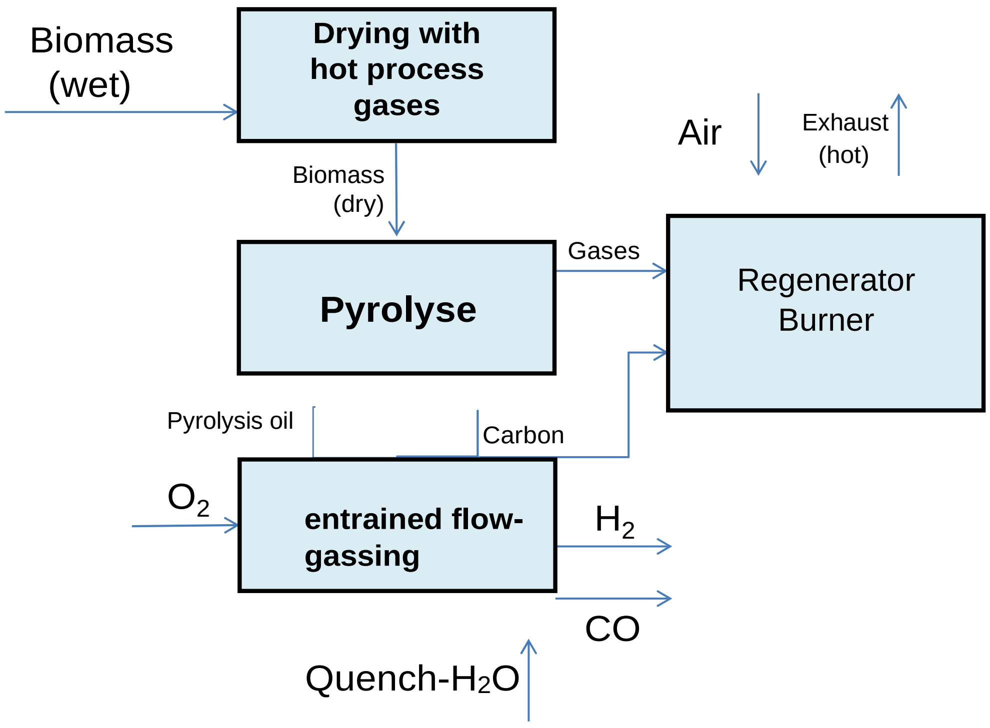


Figure 74 Process diagram biomass gasification - entrained flow

Like fluidized bed gasification, entrained flow gasification consists of several sub steps.

- the biomass (typical values for poplar according to [123]) is first dried. The modeling was analogous to the drying in fluidized bed gasification.
- Subsequently, the biomass is subjected to pyrolysis at 500 °C, forming pyrolysis oil, water, coke, ash, and pyrolysis gases with the composition given in Table 46 [154]. The pyrolysis oil and coke together form a suspension (slurry).
- For heat recovery, the resulting gases, together with a small fraction of the slurry, are burned, the amount of which depends on the heat demand to be met and was 4% of the slurry in the model. Combustion with a λ-value of 1.2 was modeled by Gibbs reactor model.
- The entrained flow gasification runs at much higher temperatures than the fluidized bed gasification, it was modeled at 1300 °C [153]. To reach this temperature, approximately 0.6 kg O2/kg slurry must be introduced. In contrast to fluidized bed gasification, this process takes place at 30 bar. Gasification was modeled using a Gibbs reactor model for thermodynamic equilibrium. In order to make the non-conventional components, such as the pyrolysis oil, accessible to a thermodynamic modeling, it was separated into the respective elements and water in a separate reactor model coupled via the heat balance. Due to the higher reaction temperatures, this produces a tar-free crude synthesis gas

consisting largely of CO, H2, CO2 and H2O.
At the end of entrained flow gasification, which has a very short residence time in the range of seconds [192], the synthesis gas is quenched to 500 °C using water.

Table 46 Product components in the pyrolysis of 1 kg biomass (dry) [154]

Components	**Mass fractions Ma.-%**
Pyrolysis oil (organic components)	59,9
Water	10,8
Carbpn	16,2
Gas	13,1

Operating materials

No operating materials were considered separately for this process except for the biomass used.

Currents

Table 47 shows the most important material and heat flows that are considered for further cost modeling.

Table 47 Overview of material and energy flows for the generation of 32 MJ synthesis gas (calorific value reference, equivalent to one liter of gasoline) in biomass gasification (entrained flow)

	ON	OFF
Material flows	Biomass*: 5,04 kg Oxygen: 1,19 kg	CO: 2,17 kg H_2: 0,0843 kg
Energy flows	Electricity: 1,95 MJ	Heat (500→400 °C): 0,778 MJ Heat (500→105 °C): 2,65 MJ

* Water content: 50 %

Capital costs

The capital costs of entrained flow gasification listed in Table 48 are generally slightly higher than those of fluidized bed gasification, depending on the source.

Table 48 Capital costs for entrained flow biomass gasification (TIC reference)

Plant size MW (biomass)	**Cost M€ (2018)**	**Refernce Year**	**spec. CAPEX €/kW (biomass)**	**Source**
389	161,1	2010	414	[149]
400	***320,5***	***2011***	***801***	[152]
10	7,3	2013	731	[192]

Comments

The use of pyrolysis oil opens a decentralized approach to entrained flow gasification, where pyrolysis oil coke slurry with significantly higher energy density than the initial biomass is produced in several smaller pyrolysis plants. This reduces transportation costs to a centralized large gasification plant (e.g., bioliq® concept [166]). Since the transport costs of the biomass used were not considered, this case is not considered separately in the model.

The entrained flow gasification showed slightly higher costs in the model compared to the modeled fluidized bed gasification, so that most of the model calculations on BtX processes presented in the study are based on fluidized bed gasification. However, this discrepancy is mainly due to the different capital costs assumed according to [152], which have a comparatively large uncertainty. Other sources assume that the capital costs are very similar [192].

Cellulose ethanol

Process

Cellulose ethanol production consists of several substeps (see Fig. 75), which are linked in the model via the respective yields of the individual steps. This allows flexible adaptation to the composition of the lignocellulose under consideration.

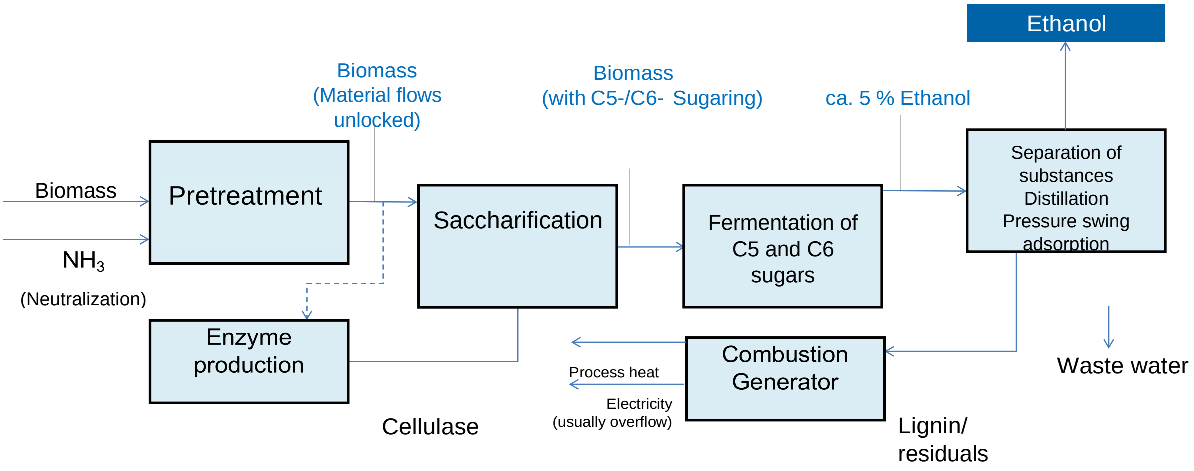


Figure 75 Process diagram - cellulosic ethanol (2G ethanol)

Three different feedstocks were considered: Corn straw, wheat straw, and poplar. The composition of the three materials is given in Table 49:

Table 49 Composition of the biomass under consideration

Components in Ma.-%	Poplar [157] [222]	Corn straw [223]	Wheat straw [224]
Moist	50	25	15
Proportions in dry biomass:	42,4	33,4	35,1
Cellulose	26,4	33,6	24,1
Hemicellulose	16,5	22,2	18,2
Xylan	1,0	4,1	1,8
Arabinan	5,0	0,6	0,7
Mannan	0,6	1,4	1,1
Galactan	3,3	5,4	2,3
Acetate	24,2	10,7	17,8
Lignin	0,6	5,9	2,7
Ash	0,0	2,2	3,5
Insoluble others	6,3	14,1	16,8

The following steps were considered (see Figure 75):

- \- The main aim of digestion is to dissolve the tightly interwoven structures of the lignocellulose in order to increase the accessibility for cleaving enzymes. In Clariant's Sunliquid® process, the lignocellulose is treated with superheated water for a certain time [225].
  In the model, the water acts on the lignocellulose at 190 °C and 12 bar [65]. The biomass fraction was assumed to be about 30% [156].
  In some cases, even a small percentage of the biomass is split [65]. In particular, acetates (components of hemicellulose) are dissolved in the form of acetic acid. This requires subsequent neutralization with ammonia. Otherwise, the digested lignocellulose would be too acidic for the subsequent steps [65].
  \- For enzyme production for the cleavage of celluloses into sugars, a side stream of the digested biomass (approx. 5%) is used as substrate [155]. In this process, mainly the contained cellulose is consumed. After enzyme production, the cellulases produced in this way are added to the saccharification process along with the unconsumed remainder.
  \- Saccharification runs at 50 °C [66]. During this process, the celluloses are hydrolytically cleaved into individual sugar monomers; according to [65], a conversion of 91.1 % was assumed.
  \- The individual sugars are fermented to ethanol in a separate fermenter, which operates at about 30 °C [66]. Special yeasts are used that can metabolize both C6 sugars (hexoses) and C5 sugars (pentoses) (in addition to the C6 sugars mannose and galactose, hemicellulose also contains the C5 sugars xylose and arabinose) [225]. Ethanol selectivities of 95% and 85% were assumed for C6 sugars and C5 sugars, respectively [65], [156].
  \- In the mass separation process, an azeotropic water-ethanol mixture is first produced with two distillation stages, from which the water is removed by a subsequent adsorption process to produce anhydrous ethanol [155]. The energy input for the material separation according to [156] is included in the model of cellulose ethanol production.
  \- The unreacted residues are thermally utilized. Lignin, which in principle cannot be converted to ethanol, is separated with other solids and burned directly. The remaining substances, which are present in relatively low concentrations dissolved in water, are converted to methane (analogous to biogas) in a fermenter (with an energetic yield of 72 % [156]). The usable energy in this process is modeled according to information on calorific values from [156] based on the residual materials resulting in the model.
  After deduction of the necessary heat energy modeled for the processes or estimated according to [156], the remaining heat energy is used for electricity generation, from which, after deduction of the necessary electricity demand [156], a significant amount usually remains, which can be sold.

Operating materials

The assumed biomass prices were 18 €/MWh for wood (poplar) [79], 31.5 €/t dry matter for corn straw [226], and wheat straw [227

As a further operating material, ammonia for the necessary neutralization was taken into account in the cost calculation. Due to the integrated enzyme production, no extra costs are incurred for enzymes.

Currents

For the three feedstocks studied: poplar, wheat straw, corn straw, the flows shown in Table 50 were determined.

Table 50 Overview of material and energy flows in the production of 1 kg of cellulosic ethanol

	EIN	AUS
Cellulose ethanol from wood		
Material flows	Biomass*: 7,64 kg Ammonia (NH_3): 35,8 g	Ethanol: 1 kg
Energy Flows	-	Electricity: 6,85 MJ
Cellulose ethanol from wheat straw		
Material flows	Biomass**: 5,24 kg Ammonia (NH_3): 29,0 g	Ethanol: 1 kg
Energy Flows	-	Electricity: 9,00 MJ
Cellulosic ethanol from corn stover		
Material flows	Biomass***: 5,60 kg Ammonia (NH_3): 64,8 g	Ethanol: 1 kg
Energy flows	-	Electricity: 1,90 MJ

* Water content: 50 %
** Water content: 15 %
*** Water content: 25 %

Capital costs

The capital costs were derived from the respective mass and energy flows passed through using the data from Humbird et al [156]. These vary depending on the composition of the lignocellulose. For the pretreatment, data for hot water treatment from Kazi et al. [65] were used in deviation.

Table 51 Capital costs used for 2G ethanol extraction for different feedstocks (TIC reference) according to data from [156] and [65].

Plant size MW (Ethanol)	Cost M€ (2018)	Reference year	spec. CAPEX€/kW (Ethanol)	Feedstock
119	177,8	2007	1499	Wood (poplar)
173	238,3	2007	1379	Wheat straw
162	212,6	2007	1314	Corn straw

The degression coefficient χ for the overall process can be estimated as 0.7 based on the data for the individual components in [156].

Water Gas Shift Reaction

Process

Water Gas Shift Reaction (WGS)

$CO + H_2O \rightleftarrows CO_2 + H_2$

enables the shift of the ratio between hydrogen and carbon monoxide in the synthesis gas. Biomass gasification produces the substances in an approximate molar ratio of 1:1 (H_2:CO). However, ratios of 2:1 or, in the case of methanation, 3:1 are required for most subsequent syntheses. In hydrogen production via WGS, 99 % of the carbon monoxide is converted [162].

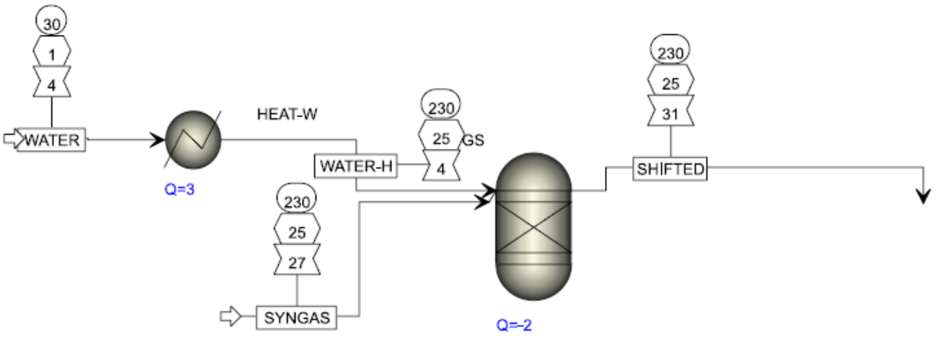


Figure 76 Flow diagram (Aspen Plus) for the water gas shift reaction prior to Fischer-Tropsch synthesis.

The process runs catalytically at 230 °C and 25 bar [128]. For hydrogen production, the temperature is 210 °C [162] since the equilibrium situation is more favorable there. The reactor is modeled as a Gibbs reactor where equilibrium is established (see Figure 76). The amount of water required for the desired conversion in each case is determined iteratively via Aspen Plus.

Operating materials

Only water is used as a fuel to shift the equilibrium. The synthesis gas comes from biomass gasification.

Currents

Table 52 Overview of material and energy flows during the water gas shift of the raw synthesis gas from biomass gasification (fluidized bed) for 32 MJ product gas each (calorific value reference, corresponds to 1 liter of gasoline equivalent)

	On	Off
	for Fischer-Tropsch synthesis (H2:CO ratio approx. 2:1)	
Material flows	CO: 1,49 kg H_2: 0,145 kg Water: 0,231 kg	CO: 1,14 kg H_2: 0,171 kg Water: 0,004 kg CO_2: 0,556 kg
Energy flows	Heat (224→230 °C): 0,003 MJ Heat (224 °C): 0,425 MJ Heat (30→224 °C): 0,222 MJ	Heat (272→230 °C): 0,180 MJ Heat (230 °C): 0,502 MJ
	for methanation (H2:CO ratio approx. 3:1)	
Material flows	CO: 1,51 kg H_2: 0,147 kg Water: 0,409 kg	CO: 0,889 kg H_2: 0,192 kg Water: 0,009 kg CO_2: 0,977 kg
Energy flows	Heat (267→300 °C): 0,124 MJ Heat (230 °C): 0,124 MJ Heat (224→230 °C): 0,005 MJ Heat (224 °C): 0,752 MJ Heat (30→224 °C): 0,394 MJ	-
	Hydrogen production (CO conversion 99%)	
Material flows	CO: 1,57 kg H_2: 0,153 kg Water: 2,21 kg	CO: 0,016 kg H_2: 0,265 kg Water: 1,21 kg CO_2: 2,45 kg
Energy flows	Heat (210 °C): 1,98 MJ Heat (30→210 °C): 1,94 MJ	Heat (210→164 °C): 0,406 MJ Heat (164→141 °C): 1,56 MJ Heat (141→109 °C): 1,18 MJ Heat (109→40 °C): 1,18 MJ

Capital costs

The capital costs of the WGS are shown in table 53. The degression coefficient χ has been assumed to be 0.67 [161].

Table 53 Capital costs used for the water-gas shift reaction (TIC reference).

Plant sizekg/s	Costs M€ (2018)	Refernce year	Source
150	9,6	2014	[161]

Comments

For direct DME synthesis from syngas, only a stoichiometric ratio of 1:1 (H2:CO) is required. The WGS can be omitted in this process since this ratio is achieved in biomass gasification.

Reverse water gas shift reaction

Process

The reverse water gas shift (rWGS)-Reaction

$CO_2 + H_2 \rightleftarrows CO + H_2O$

serves to generate the synthesis gas (a mixture of CO and H2) required for the subsequent syntheses in the respective necessary stoichiometric ratio.

The rWGS is a core element of many PtX technologies but is otherwise hardly used. Thus, there is no really established technology for rWGS. According to König [163], a relatively simple way is to use a gas-phase reactor at temperatures of at least 750 °C, at which thermodynamic equilibrium is established. This reactor must be heated due to the high temperatures and the endothermic reaction taking place inside.

Figure 77 shows the Aspen Plus flowsheet for this process, essentially the initial mixture (CO2 and H2) reacts in the rWGS reactor until thermodynamic equilibrium is reached, this also produces small amounts of the unwanted byproduct CH4. Thereafter, CO2, CH4 and H2O are separated. Part of the unreacted CO2 is recycled.

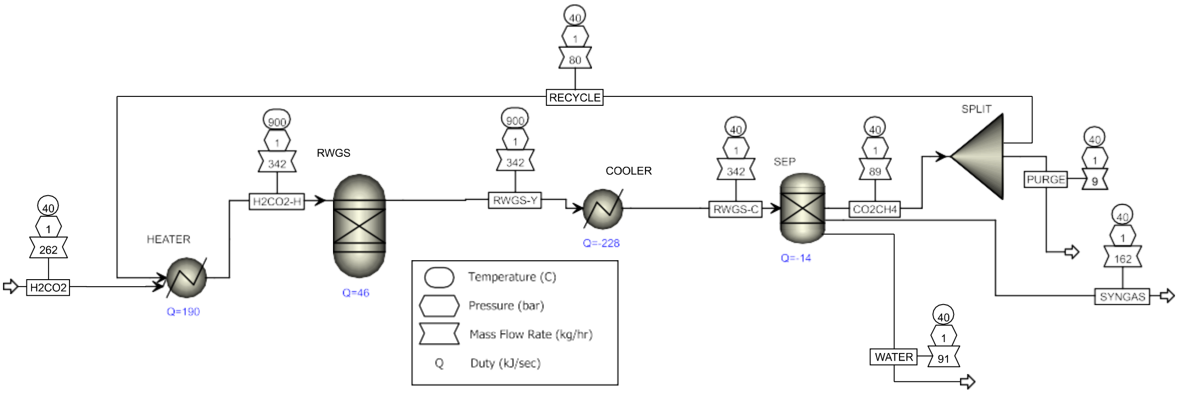


Figure 77 Flow diagram (Aspen Plus) for the reverse water gas shift reaction

An alternative to rWGS would be syntheses that do not start from CO and H2, but from CO2 and H2. Although these are part of current research projects [228], there are hardly any established technologies, which is why the use of an rWGS currently appears necessary.

Currents

Table 54 lists the incoming and outgoing material and energy flows.

Table 54 Overview of the most important material and energy flows for the generation of 1 kg of synthesis gas (for methanol synthesis) via reverse water gas shift

	On	Off
Material flows	H_2: 0,195 kg CO_2: 1,482 kg	H_2: 0,126 kg CO: 0,874 kg H_2O: 0,592 kg CO_2: 0,071 kg CH_4: 0,013 kg
Energy flows	Heat (900 °C): 0,87 MJ Heat (40→900 °C): 4,72 MJ	Heat (900→161 °C): 3,88 MJ Heat (161→100 °C): 1,48 MJ Heat (100→ 40 °C): 0,53 MJ

Capital costs

At present, hardly any commercial plants exist for rWGS. Nevertheless, estimates of capital costs can be found in the literature [164], see Table 55. The degression coefficient χ was assumed to be 0.65 [164]..

Table 55 Capital costs used for the water gas shift reaction (TIC reference)

Plant size kg/s	**Cost M€ (2018)**	**Refernce year**	**Source**
29,6	7,5	2010	[164]

Comments

Alternative routes, such as the use of iron oxide, which can act as an oxygen carrier and allow separate routing of CO2 and H2 [202] - the so-called "chemical loop" process - have not been pursued.

Methanation of CO2 and H2

Process

During methanation, methane is formed from carbon dioxide and hydrogen; this reaction is also known as the Sabatier reaction:

$CO_2 + 4\ H_2 \rightleftarrows CH_4 + 2\ H_2O$

CO2 methanation lends itself to PtX concepts because the reverse water gas shift step is not required.

The reaction is technically carried out under elevated pressure with a catalyst in a fixed bed. Suitable catalysts are metals (e.g. Ni, Co, Ru or Rh) on oxide support materials [174]. The process is relatively strongly exothermic. The technical implementation can be adiabatic or polytropic. In the following, an approach with 3 polytropically operated, cooled tube bundle reactors according to [174] was used.

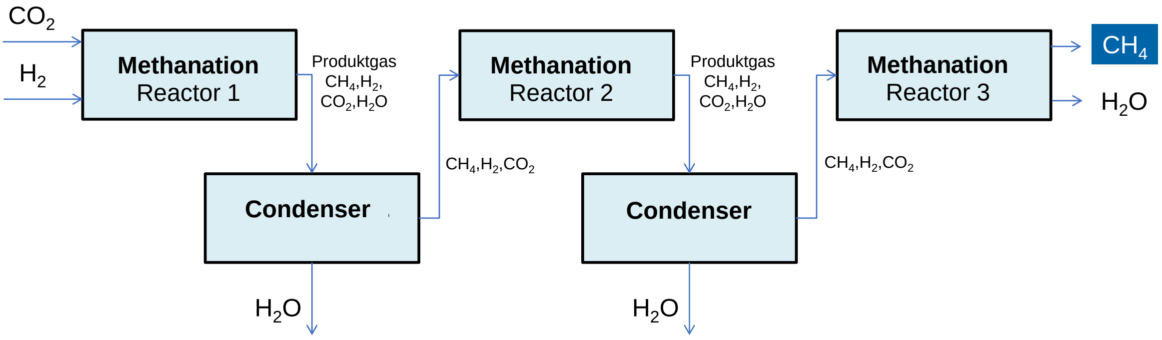


Figure 78 Process diagram - Methanation of CO2 with H2

The reactor temperatures range from 240 to 290 °C, the pressure is approx. 14 bar. Between the reactors, the product stream is cooled to 25 °C in a condenser so that the water can be condensed and removed (see Fig. 78). This shifts the equilibrium position of the methanation reaction towards methane. The conversions in the individual reactors were determined based on literature data [174]. The charge conversion is largely complete; only traces of the reactants are still contained in the methane produced.

Operating materials

For the nickel catalyst, costs of €0.42 per t/a of plant production capacity per year were estimated according to data in [175].

Currents

Table 56 Overview of material and energy flows for the production of 1 kg methane from CO2

	On	Off
Material flow	CO_2: 2,87 kg H_2: 0,507 kg	CH_4: 1 kg H_2O: 2,48 kg
Energy flow	Heat (77→253 °C): 1,84 MJ Heat (25→242 °C): 1,13 MJ Heat (25→240 °C): 0,695 MJ Heat (40→77 °C): 0,725 MJ Elektrizität: 0,060 MJ	Heat (309→253 °C): 0,013 MJ Heat (291 °C): 0,635 MJ Heat (291→115 °C): 0,574 MJ Heat (253 °C): 7,33 MJ Heat (253→154 °C): 0,877 MJ Heat (240 °C): 2,83 MJ Heat (240→142 °C): 0,454 MJ Heat (154→107 °C): 3,53 MJ Heat (142→81 °C): 1,49 MJ Heat (115→54 °C): 0,550 MJ Heat (107→25 °C): 1,65 MJ Heat (81→25 °C): 0,431 MJ Heat (54→25 °C): 0,112 MJ

Capital costs

Table 57 shows data for the capital costs of methanation via CO2. The degression coefficient χ was taken from the methanation of CO with 0.796.

Table 57 Capital costs for methanation via CO2 (TIC reference)

Plant size MW (Methane)	Cost M€ (2018)	Reference year	spec. CAPEX €/kW (methane)	Source
46	14,2	2009	307	[175]

Comments

An alternative to catalytic methanation of CO2 with H2 would be biological methanation, which could be carried out with all methane-forming microorganisms [229]. Currently, plants for the targeted biological methanation of CO2 have only a low technical maturity. The expected costs are also higher than catalytic processes. However, it might be interesting to feed H2 into biogas plants to increase the yield [229].

Methanation of CO with H2

Process

The methanation of CO with H2 proceeds analogously to the methanation of CO2 according to the following reaction equation:

$CO + 3\,H_2 \rightleftarrows CH_4 + H_2O$

The catalysts and operating conditions used are similar to those for CO2 methanation. The main difference is the smaller quantities of water, which means that the water produced does not have to be discharged during the process.

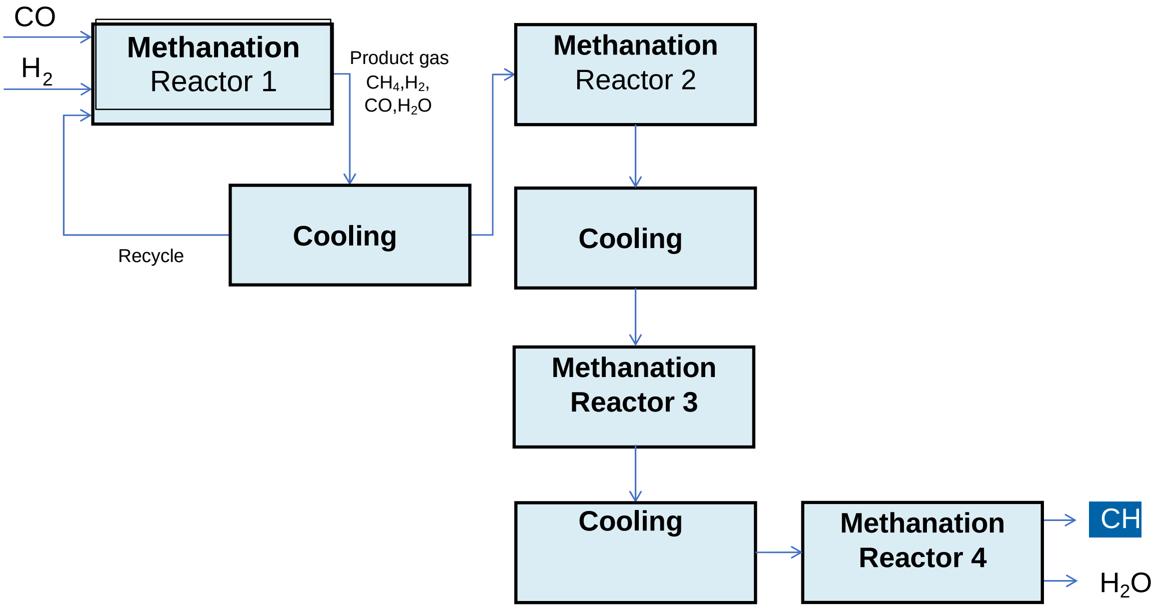


Figure 79 Process diagram - Methanation of CO with H2

The modeling based on the TREMP process [177] was carried out using 4 adiabatic reactors, which were modeled as equilibrium reactors. The inlet temperature is 300 °C in each case, and 250 °C for the last reactor. The first reactor is operated in a cycle to limit the exotherm. The cycle ratio was modeled such that the outlet temperature does not exceed 700 °C. The required cycle ratio was 3,12.

Operating materials

For the nickel catalyst, costs of €0.42 per t/a of plant production capacity per year were estimated according to data in [175].

Currents

The modeled material flows during methanation are given in Table 58. The strong exothermicity of the process can be seen.

Table 58 Overview of material and energy flows for the production of 1 kg methane from CO

	On		Off	
Material flow	CO: H_2:	1,77 kg 0,381 kg	CH_4: H_2O:	1 kg 1,08 kg
Energy flow	Electricity:	0,018 MJ	Heat (701→300 °C): Heat (700→300 °C): Heat (558→300 °C): Heat (419→250 °C): Heat (298→81 °C): Heat (81→7 °C): Heat (57→25 °C):	8,34 MJ 2,67 MJ 1,61 MJ 0,970 MJ 1,09 MJ 2,16 MJ 0,722 MJ

Capital costs

The cost of capital reported in Table 59 yields a degression coefficient χ of 0.796.

Table 59 Capital costs for methanation via CO (TIC reference)

Plant size MW (Methane)	Cost M€ (2018)	Reference Year	spec. CAPEX €/kW (methane)	Source
67	***20,0***	***2016***	***300***	[178]
205	49,0	2016	238	[178]

Fischer-Tropsch-Synthesis

Process

In the Fischer-Tropsch synthesis, a broad spectrum of hydrocarbons is produced from synthesis gas according to the general reaction equation.

$CO + 2\,H_2 \rightleftarrows -CH_2- + H_2O$

The term -CH2- stands for a part of a hydrocarbon chain. For the most part, unbranched kerosenes, olefins and oxygenates are formed in a wide range of chain lengths (see Fig. 36 on p.59). The exact product composition can be influenced by the choice of process conditions and catalyst.

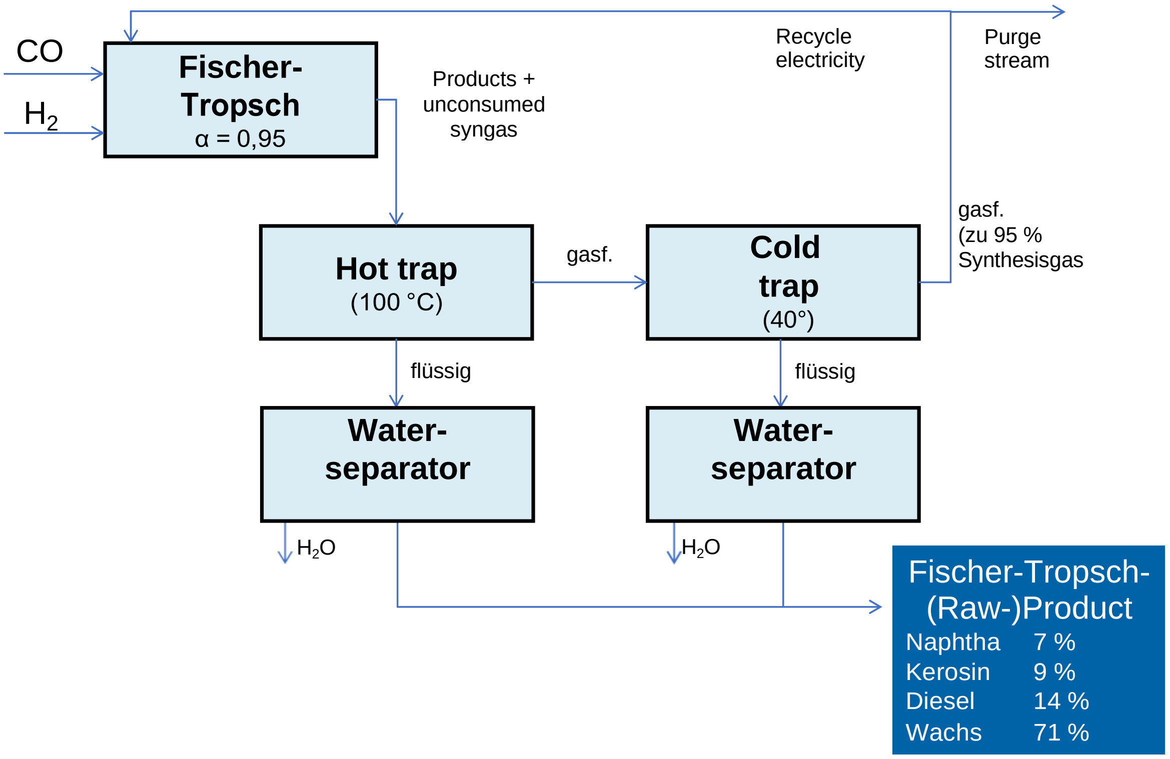


Figure 80 Process diagram - Fischer-Tropsch synthesis

In the model, a conversion in the reactor of 15 % of the carbon monoxide was assumed for the Fischer-Tropsch synthesis. The conversion of CO in the reactor is increased to a total of 95 % by recycling unreacted reactants (see Figure 80) [167]. In the model, only the conversion to n-paraffins was considered, whose chain lengths follow an Anderson- Schulz-Flory distribution. For the modeling, a high chain growth probability α of 0.95 was applied [167], [168], which can be achieved with a LTFT synthesis (low-temperature Fischer-Tropsch synthesis - low temperature Fischer Tropsch synthesis) on cobalt catalysts [167], [230]. The reaction temperature is 220 °C [231], the process pressure 40 bar. Primarily products in the wax range are formed (see Fig. 80).

The gaseous products, which also include the unreacted synthesis gas, are separated from the liquid products via a hot trap (100 °C) and a cold trap (40 °C) and recycled to increase yield.

Operating materials

Besides the H2 and CO used, no other fuels were modeled separately.

Currents

The material flows are summarized in Table 61 on p. A5.26 for the Fischer-Tropsch synthesis including upgrading.

By-products

In addition to the target products in the middle distillate range, products are also formed in the boiling range of naphtha. These mainly branched and unbranched kerosenes are suitable, for example, as feedstock for olefin production in a steam cracker [231]. The gaseous products produced in small quantities are thermally recycled.

Capital costs

For the Fischer-Tropsch synthesis, together with the upgrading described in the following chapter, the capital costs shown in Table 60 were determined. The highlighted values were used for the model. The degression coefficient χ is given as 0.72 according to [166].

.

Table 60 Capital costs for Fischer-Tropsch synthesis incl. upgrading (TIC reference)

Plant size MW (FT-Product)	Cost M€ (2018)	Reference Year	spec. CAPEX €/kW (FT-Product)	Source
193	***85,6***	***2010***	***444***	[149]
306	100,7	2005	329	[232]

Comments

Fischer-Tropsch synthesis can be carried out in many different process and reaction configurations. Different catalysts and temperatures can lead to completely different product spectra. For the model, LTFT with cobalt catalyst was chosen with the aim of obtaining a high middle distillate yield [168].

Upgrading Fischer-Tropsch products - Hydrocracking

Process

The Fischer-Tropsch synthesis, see previous section, yields a large amount of long-chain n-paraffins, largely in the boiling range of waxes (C - number >22). Hydrocracking allows the larger molecules to be hydrogenated into smaller ones, predominantly in the middle distillate range. As a desirable side reaction, isomerization of the originally largely unbranched hydrocarbons takes place.

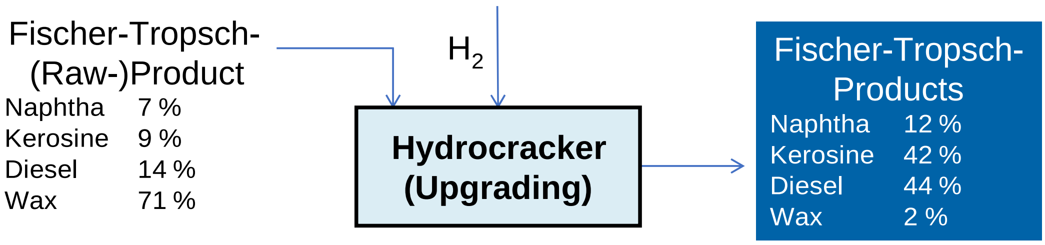


Figure 81 Process diagram - Upgrading Fischer-Tropsch products

Hydrocracking takes place in the fixed-bed reactor at 290 °C, a pressure of 40 bar and an H2-to-feed ratio of 750 m³ i.N./m³. The kinetics according to [179] for a catalyst consisting of Pt on amorphous aluminosilicate was implemented in the model and leads to the product distribution shown in Figure 81.

Operating materials

The hydrogen required for hydrocracking is taken from the synthesis gas. This quantity must be considered when setting the (reverse) water gas shift reaction. Apart from this, no other operating materials had to be taken into account.

Currents

Table 61 shows the material and energy flows.

Table 61 Overview of material and energy flows for the production of 1 kg Fischer-Tropsch middle distillate

	EIN Maintenance	AUS
Material flow	Fischer-Tropsch-Synthesis:CO: 2,53 kg H_2: 0,373 kg Upgrading: H_2: 0,0063 kg	Middle distillates: 1,00 kg Naphtha: 0,14 kg LPG: 0,01 kg H_2O: 1,54 kg
Energy flow	Heat (100→290 °C): 0,756 MJ Heat (13→220 °C): 10,0 MJ Heat (9→100 °C): 0,039 MJ Electricity: 0,461 MJ	Heat (1600→120 °C): 5,67 MJ Heat (290 °C): 0,100 MJ Heat (277→100 °C): 0,002 MJ Heat (270→220 °C): 0,407 MJ Heat (220 °C): 13,9 MJ Heat (220→100 °C): 6,72 MJ Heat (113→71 °C): 4,59 MJ Heat (71→10 °C): 3,83 MJ

By-products and capital costs

s. By-products and capital costs Fischer-Tropsch synthesis sections on p. A5.25.

Methanol synthesis

Process

Methanol synthesis is an established large-scale process that produces more than 100 million tons of methanol annually (as of 2020 [233]). Global production capacity has more than doubled in the last 10 years. Methanol synthesis requires a ratio in the syngas of approximately 2:1 (H2:CO). Methanol synthesis also uses a certain amount of CO2 to maintain the activity of the catalyst and increase the conversions [234].

$$2\ H_2 + CO \rightarrow CH_3OH$$

The process runs on Cu/ZnO/Al2O3 catalysts at temperatures of approx. 270 °C and pressures of 50 to 100 bar. Due to the thermodynamically determined low conversions of at most approx. 40 %, the process is operated in a cycle. The synthesis gas is separated from the methanol and recycled. The purging flow is adjusted in such a way that a recycle ratio of 4 can be realized.

In Aspen Plus, methanol synthesis was modeled at 260 °C and 60 bar.

Operating materials

The catalyst was considered as the operating material. According to data in [123], the costs for this amount to € 0.35 per t/a of production capacity per year.

Currents

The main incoming and outgoing material and energy flows are listed in Table 62.

Table 62 Overview of the most important material and energy flows in the production of 1 kg of methanol from synthesis gas

	On		Off	
Material flow	H_2: CO: CO_2:	0,148 kg 0,861 kg 0,143 kg	MeOH: H_2O:	1 kg 0,043 kg
Energy flow	Electricity:	0,38 MJ	Heat (260 °C): Heat (92→40 °C):	2,664 MJ 1,748 MJ

Capital costs

Table 63 provides an overview of the range of capital costs found in the literature. A medium value was chosen for the model. A standard value of 0.6 was used as the degression coefficient χ for methanol synthesis according to [125] was used.

Table 63 Capital costs for methanol synthesis (TIC reference)

Plant sizeMW (Methanol)	Cost M€ (2018)	Reference year	spec. CAPEX €/kW (Methanol)	Source
222	16,2	2007	73	[123]
193	45,1	2001	233	[90]
216	***42,4***	***2010***	***196***	[172]
253	24,3	2009	96	[169]
304	103,2	2016	339	[170]
549	141,0	2002	257	[171]

Direct DME synthesis from synthesis gas

Process

DME synthesis from synthesis gas is basically analogous to methanol synthesis. The main difference is that the catalyst system is supplemented by an acid component which catalyzes the further conversion of methanol to DME (e.g., the zeolite H-ZSM5 [235]).

In contrast to methanol synthesis, a syngas ratio of about 1:1 (H2:CO) can be used instead of 2:1 [166], CO2 is produced as a by-product and much less H2O, which would be problematic at higher concentrations. As a result, the purified synthesis gas produced during biomass gasification can be used directly.

The following reactions take place:

Methanol Synthesis: $2\ CO + 4\ H_2 \rightarrow 2\ CH_3OH$

DME-Synthesis: $2\ CH_3OH \rightarrow CH_3\text{-}O\text{-}CH_3 + H_2O$

Water gas-Shift: $CO + H_2O \rightarrow CO_2 + H_2$

in sum:

DME from syngas (1:1): $3\ CO + 3\ H_2 \rightarrow CH_3\text{-}O\text{-}CH_3 + CO_2$

A slightly modified model of the methanol synthesis described here was used as the model. The stoichiometry of the input substances was changed and dimethyl ether was integrated as an additional possible component for the reactor. Subsequently, the unreacted synthesis gas and the intermediate methanol are recycled. In PtX processes, the CO2 is separated and used as feedstock in the reverse water gas shift. As in methanol synthesis, a cycle ratio of 4 is set.

Operating materials

Annual costs of € 1.69 per t/a production capacity were estimated for the catalyst, based on the costs of the DME synthesis catalyst together with those of the methanol catalyst. The fact that the DME catalyst has a shorter service life was taken into account.

Currents

Table 76 lists the modeled flows in the DME synthesis.

Table 64 Overview of the most important material and energy flows in the production of 1 kg of dimethyl ether from synthesis gas

	On	Off
Material flow	H_2: 0,162 kg CO: 1,66 kg CO_2: 0,275 kg	DME: 1 kg H_2O: 0,166 kg CO_2: 0,721 kg
Energy flow	Heat (15→58 °C): 0,840 MJ Heat (58→68 °C): 0,134 MJ Electricity: 0,430 MJ	Heat (260 °C): 5,10 MJ Heat (101→10 °C): 2,10 MJ

Capital costs

Due to the similarities of DME synthesis from syngas to methanol synthesis, their capital costs are also very similar [171], so that the assumed capital costs of methanol synthesis were also used analogously for DME synthesis.

Methanol-to-Gasoline-Process

Process

Methanol can be converted very selectively into a high-quality gasoline component by the methanol-to-gasoline (MtG) process. In the process, the methanol is converted using zeolite catalysts at 330 °C and 14.5 bar. The exothermic process is cooled to run at one temperature level. Components in the gasoline range are produced with a selectivity of about 82% [123]. The methanol is fully converted, and gaseous hydrocarbons are formed as a byproduct, some of which are used thermally or also form a value product as LPG. For the modeling, a conversion of methanol to heptane and toluene was assumed for simplicity.

Operating materials

The annual cost of the catalyst is €6.62 per t/a of plant capacity [123].

Currents

Table 65 shows the modeled material and energy flows of the MtG process including by-products.

Table 65 Overview of the most important material and energy flows in the production of 1 kg MtG gasoline

	EIN	AUS
Material flow	MeOH: 2,79 kg CO: 1,66 kg CO_2: 0,275 kg	MtG-Benzin: 1 kg LPG: 0,121 kg H_2O: 1,57 kg
Energy flow	Heat (150→330 °C): 1,02 MJ Heat (150 °C): 2,59 MJ Heat (40→150 °C): 1,04 MJ Electricity: 0,015 MJ	Heat (1876→110 °C): 4,03 MJ Heat (400 °C): 4,36 MJ Heat (400→183 °C): 1,40 MJ Heat (183→169 °C): 3,63 MJ Heat (169→32 °C): 1,48 MJ

Capital costs

The capital costs for the MtG process are shown in Table 66. The estimate for Nordic Blue Crude's PtL plant built in Norway with CAC's MtG process [133] was used. A learning curve was assumed for a modeled nth plant[20].

The degression coefficient χ was assumed to be 0.6, the default value for many chemical processes according to [125].

---

[20] Assuming a moderate learning rate of 15% per twice the plant capacity [243], half the investment cost of a new plant would be expected at 20 times the installed capacity.

Table 66 Cost of capital for MtG processes (TIC reference)

Plant size MW (MtG-Benzin)	**Cost M€ (2018)**	**Reference Year**	**spec. CAPEX €/kW (MtG-Benzine)**	**Source**
52	30,1	2016	580	[178]
134	56,8	2016	424	[178]
60	34,8	2016 - 1st plant	585	[133]
60	***17,4***	***n-th plant (estimation)***	***292***	Estimated from [133]
187	58,2	2009	312	[169]
246	21,2	2007	86	[123]

DME Synthesis from methanol

Process

In DME synthesis from methanol, the latter is converted to dimethyl ether (DME) over an acid catalyst.

$2\ CH_3OH \rightarrow CH_3\text{-}O\text{-}CH_3 + H_2O$

According to [182], the reactor inlet temperature in the adiabatically modeled reactor is 232 °C, the pressure is 10 bar. The conversion after one run is 85 % [182].

Subsequently, the DME is separated from the methanol and water by distillation at reaction pressure, and subsequently, at normal pressure, the water is separated from the methanol. The methanol is returned to the reaction to increase the yield.

Operating materials

According to data in [236], the annual cost of a zeolitic catalyst is €0.99 per t/a of production capacity.

Currents

Table 67 shows the material and energy flows.

Table 67 Overview of the most important material and energy flows in the production of 1 kg DME from methanol

	On	Off
Material flow	MeOH: 1,40 kg	DME: 1 kg H_2O: 0,427 kg
Energy flow	Heat (159 °C): 0,302 MJ Heat (139→232 °C): 0,294 MJ Heat (139 °C): 1,66 MJ Heat (117 °C): 0,524 MJ Heat (46→139 °C): 0,516 MJ Electricity: 0,0004 MJ	Heat (359→149 °C): 0,735 MJ Heat (149→88 °C): 1,28 MJ Heat (81 °C): 0,672 MJ Heat (46 °C): 0,685 MJ

Capital costs

Table 68 shows data for the capital costs of DME synthesis from methanol. The comparatively less complex process step has rather low costs. The degression coefficient χ was assumed to be 0.6 as the standard value for chemical processes according to [125] was assumed.

Table 68 Capital costs for methanation via CO2 (TIC reference)

Plant size MW (DME)	Cost M€ (2018)	Reference Year	spec. CAPEX €/kW (DME)	Source
194	9,3	2011	48	[182]

OME-Synthesis

Process

The classical OME synthesis consists of four sub steps [184] (see Figure 82), each of which was modeled separately:

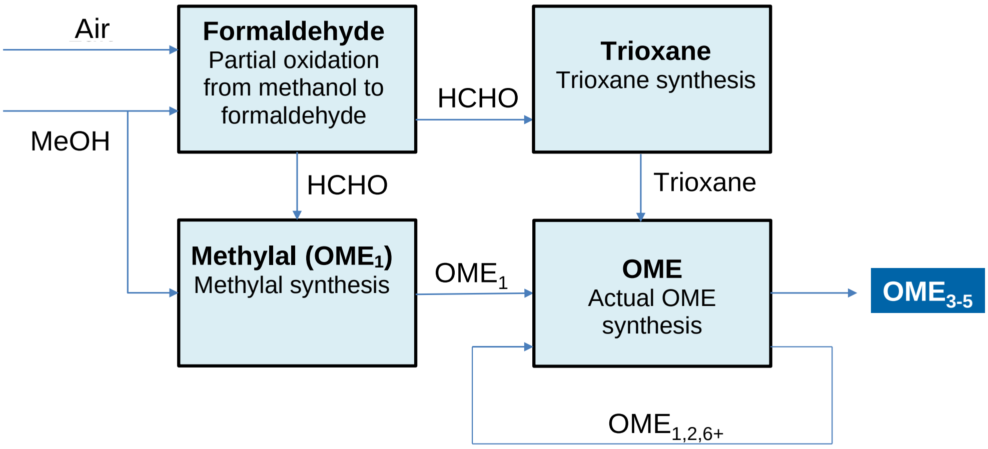


Figure 82 Process diagram - OME synthesis

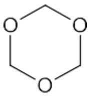
- First, part of the methanol is partially oxidized to formaldehyde:

  $CH_3OH + ½ O_2 \rightarrow HCHO + H_2O$

  The reaction takes place in the shell-and-tube reactor on iron-molybdenum catalysts or silver catalysts [237], the inlet temperature is 200 °C, the outlet temperature 300 °C despite cooling. The pressure is 1.3 bar [186]. The necessary oxygen is added in the form of air. The molar oxygen-to-methanol ratio was 2.85. It is thus well above the stoichiometrically required value of 0.5; oxygen is added in excess. According to data on industrial processes [186], the formaldehyde selectivity of the process is slightly more than 90%, with the remainder reacting further to form undesirable carbon oxides (CO or CO2). The methanol is almost completely converted in the reactor. Subsequently, the formaldehyde is separated from the gas stream via a water scrubber [237]. The formaldehyde solution is then concentrated by distillation so that a mass fraction of 37 % formaldehyde is achieved.
- The other part of the methanol reacts with the formaldehyde to form methylal, which is an oxymethylene ether (with n=1).

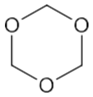
  $2\ CH_3OH + HCHO \rightarrow CH_3\text{-}O\text{-}CH_2\text{-}O\text{-}CH_3 + H_2O$

  For methylal synthesis by reactive distillation, the material and energy balance according to [187] was used.
- Part of the formaldehyde reacts to form the ring-shaped trioxane, which is a defined compound of three formaldehyde molecules. It is also stable in the anhydrous state.

3 HCHO →


This reaction takes place at 80 to 90 °C catalyzed by sulfuric acid [188], and only part of the formaldehyde is converted. The trioxane is then extracted with benzene in the model [189]. The benzene is then separated from the trioxane by distillation. A certain part of the benzene must be renewed in the process.

- In the actual OME synthesis, the methylal reacts with the trioxane to form the various oxymethylene ethers (OMEs).

  (n-1)/3  + $CH_3\text{-}O\text{-}CH_2\text{-}O\text{-}CH_3 \rightarrow CH_3\text{-}O\text{-}[\text{-}CH_2\text{-}O\text{-}]_n\text{-}CH_3$

  Acid catalysts such as acid ion exchange resins are used. The trioxane ring is opened, and it is subsequently inserted into the methylal in its entirety, or split into formaldehyde, to form an oxymethylene ether with n>1 [190]. The different OMEs are in equilibrium with each other, which depends on the process conditions and the ratio between trioxane and methylal. The model uses the underlying kinetics according to [190] to reproduce the OME synthesis. Methylal (OME1), OME2 and OME6+ are separated by distillation and recycled.

  The presence of water leads to the formation of hemiacetals and should be avoided [190]. Other possible by-products are DME and methyl formate.

The product consists essentially of OME3 to OME5 with the composition given in Table 69. In this case, it has a calorific value of 19.2 MJ/kg and a density of 1058 g/l.

Table 69 Product composition of the OME mixture (modeled)

	Mass fraction Ma.-%
OME_3	45,7
OME_4	32,3
OME_5	21,4
OME_6	0,6

Operating materials

Methanol is used as the reactant for the overall process. The benzene used in the extraction of trioxane must be permanently renewed in parts.

Currents

Table 70 shows the flows in OME synthesis, the number of modeled energy flows is relatively large due to the many partial synthesis steps.

Table 70 Overview of the most important material and energy flows in the production of 1 kg OME3-5 from methanol

	On	Off
Material flow	MeOH: 1,26 kg H_2O: 1,61 kg	OME_{3-5}: 1 kg H_2O: 2,55 kg
Energy flow	Heat (401 °C): 1,08 MJ Heat (238 °C): 4,52 MJ Heat (114 °C): 1,13 MJ Heat (101 °C): 1,06 MJ Heat (71→200 °C): 0,171 MJ Heat (71 °C): 0,880 MJ Heat (59 °C): 1,13 MJ Heat (40→200 °C): 1,68 MJ Heat (40→71 °C): 0,083 MJ	Heat (300 °C): 2,74 MJ Heat (300→120 °C): 2,20 MJ Heat (287 °C): 0,760 MJ Heat (280→188 °C): 0,157 MJ Heat (188→162 °C): 0,336 MJ Heat (173→153 °C): 0,535 MJ Heat (168 °C): 3,15 MJ Heat (162→40 °C): 0,237 MJ Heat (153→80 °C): 0,484 MJ Heat (90 °C): 0,299 MJ Heat (90→87 °C): 0,010 MJ Heat (87→74 °C): 1,37 MJ Heat (80 °C): 0,007 MJ Heat (74→7 °C): 1,65 MJ Heat (67 °C): 0,247 MJ Heat (50 °C): 1,12 MJ Heat (42 °C): 0,711 MJ Heat (7 °C): 0,399 MJ

Capital costs

Table 71 presents data for the capital cost of OME synthesis. The coefficient of degression χ was estimated to be 0.65 for somewhat more complex chemical plants according to [125] estimated.

Table 71 Capital costs for methanation via CO2 (TIC reference)

Plant size MW (OME)	Costs M€ (2018)	Reference Year	spec. CAPEX €/kW (OME)	Source
665	289,9	2016	436	[129]

Attachment 6

Modeling of heat flows and cooling demand - technical appendix

The heat flows generated by the processes and the heat demand required in the process were compared by means of a PINCH analysis so that as large an amount of the heat demand as possible could be covered by energy generated in the process. A minimum temperature difference of 5 K between the hot and cold streams was specified.

This modeling results in the necessary heat quantities that are additionally required in the process and the heat quantities that are generated, depending on the temperature level, the heat flow is used or must be passively or actively cooled [153]:

- **up to 40 °C**: Active cooling via ammonia adsorption cooling [153]. For every 1 MJ of heat supplied, 0.34 MJ of heat from the stream to be cooled is removed [238]. A capital cost of €500 is required per kW of cooling capacity [239].
- **40 to 60 °C**: Active water cooling [153], with cooling water included at a price of 0.086 €/m³ [129]. One kW of cooling capacity has a capital cost of 20 € [240].
- **60 to 100 °C**: Passive air cooling. Here, a capital cost of 20 € [239] is required.
- **100 to 250 °C**: These heat flows can be used to provide heat (also to sell heat). A utilization rate of 95 % was assumed.
- **250 to 500 °C**: The heat can be used to drive steam turbines, which can generate electricity. The efficiency for heat from this temperature range was assumed to be 60 %.
- **500 °C and above**: The heat in this range generally arises from combustion processes and is converted in the model to electricity with an efficiency of 65 % using a gas turbine. The capital costs for steam and gas turbines were taken from [149]

Attachment 7

Transport - technical annex

The transport of hydrogen and liquid products was modeled on the basis of data from the IEA [143]. The modeled CAPEX and OPEX were then used to determine the respective transport costs using the methodology described in section 6.2.

The following modules for transport components were integrated, which are described below:

- For hydrogen:
    - o Liquefaction
    - o Marine transport (incl. import and export terminals)
    - o Truck transport
    - o pipeline
    - o distribution via pipeline network
- For liquids: (diesel, gasoline, methanol, ethanol, OME).
    - o Marine transportation (incl. import and export terminals)
    - o Truck transpor

Hydrogen liquefaction

The capital costs for a plant with a capacity of 260,000 t/a are the equivalent of 1250 M€2019 according to [143]. The degression coefficient was estimated at 0.69 - a value for air separation plants [241].

Hydrogen liquefaction is relatively energy intensive. Bossel et al [141] indicate a decreasing energy requirement as plant size increases. The relationship shown therein, for advanced plants, can be described with the following equation:

$$E = 18{,}60 + 96{,}04 \cdot \exp(-0{,}8249 \cdot \log_{10} \dot{m})$$

> E is the energy required for liquefaction in % of the energy content (calorific value) of the liquefied hydrogen (141.8 MJ/kg)
>
> $\dot{m}$ is the throughput mass flow of the hydrogen in kg/h (as a measure of the plant capacity)

In addition, further OPEX costs of 4 % of CAPEX per year are to be applied [143]. The plant lifetime was assumed to be 30 years.

An alternative to liquefaction would be the use of LOHC (*liquid organic hydrogen carriers*), substances that can absorb hydrogen before transport and release it again for use. In this process, the substance itself is converted - hydrogenated and dehydrogenated. Aromatics, such as toluene, are particularly suitable for this purpose; they absorb several hydrogen molecules during conversion to naphthenes (in the case of toluene: methylcyclohexane) and can release them again during reconversion.

Marine transport (incl. import and export terminal) - Hydrogen

For ship transportation, three interrelated models were considered in principle (ship, import terminal, export terminal):

Ship

The hydrogen is transported in liquid form at a temperature of -252 °C, which requires special ships with insulated tanks. The framework data for the modeling are listed in Table 72.

Table 72 Model data used for ship transport of H2 [143]

Marine transport for hydrogen (liquid)	**Values for modeling**	
CAPEX		$M€_{2019}$/Schiff
Capacity		t H_2/Schiff
Fuel requirement full	1487	MJ/km
empty	1381	MJ/km
average speed		km/h
Flashrate		%/Filling
Evaporation rate		%/Day
else. OPEX		%(CAPEX)/a
Operating time		Year

The flash rate denotes the amount of liquid hydrogen that evaporates per filling. The evaporation rate indicates the amount of evaporation necessary to maintain the temperature in the ship's tanks by evaporative cooling. The evaporated hydrogen can be captured and is sufficient to propel the ship. For the return voyage, it was assumed that heavy fuel oil is used, with a cost of 300 €/t [242]. A total of 3 days per transport was assumed as the laytime.

Terminals

The import and export terminals were dimensioned so that hydrogen from 10 production plants can be shipped. The values used for the modeling are listed in Table 73.

The required number of tanks is derived from the capacity needed to load a ship with additional capacity resulting from the lead time.

Table 73 Model data used for terminals (ship transport) for H2 (according to [143] or own assumptions)

Terminals for hydrogen (liquid)	**Export terminal Values for remodeling**		**Import terminal Values for remodeling**	
CAPEX	259	M€$_{2019}$/Tank	286	M€$_{2019}$/Tank
Capacity	3190	t H_2/Tank	3550	t H_2/Tank
Flashrate	0,1	%/Filling	0,1	%/Filling
Fuel consumption	0,1	%/Day	0,1	%/Day
Driver	7	Days	20	Days
Travel time	0,61	kWh/kg	0,2	kWh/kg
average speed	4	%(CAPEX)/a	4	% (CAPEX)/a
other OPEX	30	Years	30	Years

Truck transport - hydrogen and liquid energy carriers

Truck transport is modeled using the data given in Table 74. Diesel fuel was assumed as the fuel (cost in the model €1.05/l). A flash rate of 1% was assumed for the transport of hydrogen.

Table 74 Model data used for truck transport ([143], [137], own assumptions).

Truck transport hydrogen (liquid) and liquids	**Export terminal values for modelingg**	
CAPEX	0,165	M€$_{2019}$/Lkw
Capacity	35	m^3
Flashrate	1,0	%/ Filling (hydrogen only)
Fuel consumption	1220,1	MJ/100 km
Driver	20,5	€/h
Travel time	45	h/Weeks
average speed	50	km/h
other OPEX	12	% (CAPEX)/a
Operating time	12	Years

Pipeline transport - hydrogen

As with the import and export terminals, it is assumed here that a pipeline transports the hydrogen from 10 plants.

For the transport of hydrogen via pipelines, a compressor station was provided every 150 km [141] to compensate for the pressure loss occurring over the previous leg. The compressor stations are operated with the transported medium - in this case hydrogen. The basic assumptions are listed in Table 75.

Table 75 Model data used for pipeline transport of H2

Pipeline transport Hydrogen (gaseous)	**Values for modeling**		**Source/Comments**
CAPEX	$0{,}004 \cdot d^2 + 0{,}6 \cdot d + 329$	€/m	[243] d: Diameter in mm
Utilization rate	75	%	[143]
Pressure	100	bar	[143]
Velocity in pipeline	ca. 5–15	m/s	Must be optimized for individual case
Pipeline roughness (→ pressure loss)	0,0015	mm	Acceptance

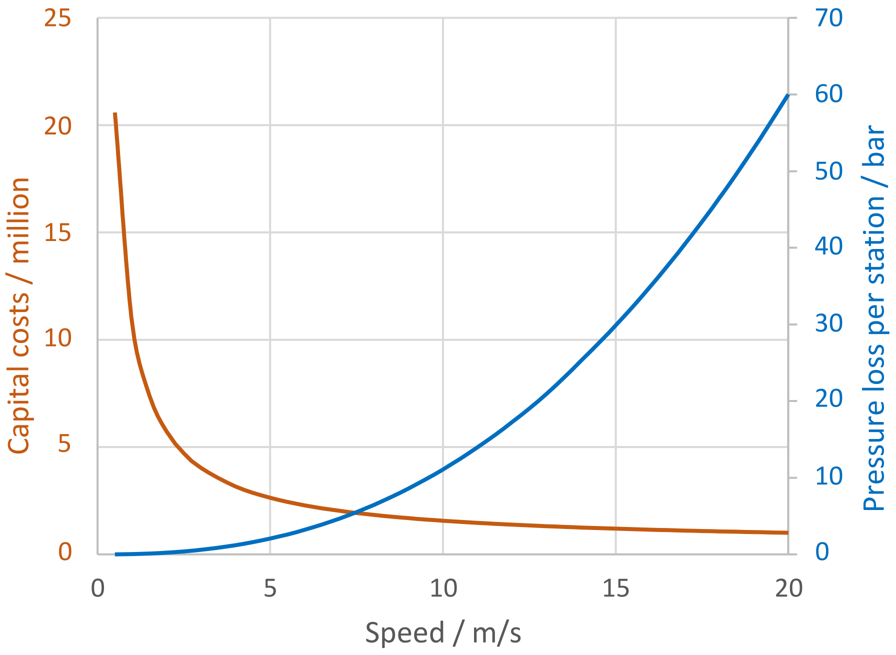


Figure 83 Characteristics for a pipeline (capacity approx. 350,000 7/a H2) as a function of the velocity of the medium (modeled).

The speed at which the hydrogen moves through the pipeline is influenced by the diameter of the pipeline. The larger the diameter, the lower the velocities

velocities are required to move the hydrogen, but the greater the capital cost (see Figure 83). The higher the velocity, the higher the pressure drop between compressor stations (see Figure 83), and the higher the cost of compression.

An optimum exists between capital costs and operating costs (for energy expenditure of the compressors), which was determined depending on the basic conditions. Important influencing variables in this design are the length of the pipeline, the volume flow to be transported and the cost of the hydrogen.

Distribution network - hydrogen

For distribution, a distribution network was modeled analogously to long-distance transport by pipeline. Due to the shorter length, no compressor stations are necessary. Smaller networks branch off from the large distribution network, which can bring the hydrogen to the final consumers; their costs must also be considered. The pressure in these networks is significantly lower.

Table 76 Model data used to model an H2 distribution network. [143]

Distribution network Hydrogen (gasf.)	**Values for modeling**	
CAPEX	$0{,}0034 \cdot d^2 + 0{,}6 \cdot d + 329$	€/m d: Diameter in mm
Utilization rate	100	%
Print	80	bar
Branching networks Length Flow CAPEX Pressure	3 365 300 10	km t/a €/m bar

The modeled costs refer to a new construction of the networks. It should be noted here that hydrogen networks already exist in some cases. In addition, the use of natural gas infrastructure with H2 as an admixture in natural gas is possible. If these possibilities exist, the distribution of hydrogen could be relatively inexpensive.

Marine transport - liquid energy carriers

The approach to modeling the marine transport of liquid energy carriers is the same as for the transport of liquid hydrogen. However, unlike the transport of liquid hydrogen, there is no loss due to evaporation when transporting liquids. The CAPEX for the ships is significantly lower, but due to the larger transported mass, more fuel per km is required Table 77).

Table 77 Model data used for ship transport of liquids [143]

Ship transportation for liquids	**Values for modeling**	
CAPEX		M€$_{2019}$/Schiff
Capacity		m^3/Schiff
Fuel requirement full	3300	MJ/km
empty	1381	MJ/km
average speed		km/h
other OPEX		%(CAPEX)/a
Operating time		Jahre

Import and export terminals were modeled with data given in table 78.

Table 78 Model data used for terminals (marine transport) for liquids [143]

Terminals for liquids	**Export terminal values for modeling**		**Import terminal values for modeling**	
CAPEX	31	M€$_{2019}$/Tank	31	M€$_{2019}$/Tank
Capacity	71620	m^3/Tank	85253	m^3/Tank
Lead time	7	Days	20	Days
Electricity demand	0,01	kWh/kg	0,01	kWh/kg
Other OPEX	4	%(CAPEX)/a	4	%(CAPEX)/a
Operating time	30	Years	30	Years

Attachment 8

Calculation of electricity demand for sector coupling

Road vehicles - electromobility

The calculations of the electric energy demand for the complete replacement of combustion engines in road vehicles by electric drives are based on the current fuel consumption (2016: diesel fuel 37.9 million tons, gasoline fuel 18.2 million tons [244]) in conjunction with the so-called tank-to-wheels efficiencies of the different drive types. These efficiencies take into account the losses in the vehicle during the conversion of the absorbed energy (fuel, electrical energy) into the kinetic useful energy.

In contrast to other projections, which are based on estimated driving distances and specific, average electric energy consumption mostly of small cars, this estimate is based on real energy demand in road traffic.

The amount of electricity required for substitution is calculated as follows

$$\text{Electricity demand} = m_{\text{Fuel}} \cdot Q_{i,\ \text{Fuel}} \cdot \frac{\eta_{\substack{\text{Internal combustion}\\ \text{engine}}}}{\eta_{\text{Electric}}}$$

with	m_{fuel}	Fuel requirement,
	$Q_{i,\text{fuel}}$	Specific energy content (calorific value) of the fuel
	η	Well-to-wheels efficiencies

The following average tank-to-wheels efficiencies were used:

- Diesel cars 30%, diesel trucks 40%.
  (Assuming that 50 % of diesel fuel is used in cars and 50 % in trucks, the average efficiency of diesel drives is 35 %),
- Gasoline car 25 %,
- electric car 78 %
  (Engine efficiency incl. power electronics 90 %, charge/drain losses traction battery 20 %, not considered: Losses due to self-discharge)

Example: Electricity demand for diesel fuel substitution:

$$= 37{,}9\ 10^9\ \text{kg} * 43\ \text{MJ/kg} * 0{,}35 / 0{,}78 = 731{,}3\ \text{GJ} = 203\ \text{TWh}$$

Aviation - synthetic electricity-based fuels

There is a consensus that liquid fuels will continue to be indispensable for aviation in the future. From the point of view of sector coupling, a synthesis of turbine fuels based on carbon dioxide and hydrogen produced by means of water electrolysis ("PtL" = power-to-liquid) can be considered.

In calculating the electricity requirement, it is assumed that carbon dioxide is available and that no energy expenditure is required in this respect. The electricity requirement then results only from the electrolysis to provide the hydrogen.

For kerosene synthesis, the hydrogen demand can be estimated using the following stoichiometric equation:

$CO_2 + 3\ H_2 \leftrightarrow -CH_2- + 2\ H_2O$

Here, -CH2- stands for the chain links of the aliphatic hydrocarbons of the products.

With a demand for Jet A1 in 2016 of 9.2 million metric tons, 28.85 million metric tons of carbon dioxide must be converted (corresponds to a C quantity of 7.87 million metric tons). This requires 3.93 million tons of hydrogen according to the above equation. With a calorific value of hydrogen of 39.69 MWh/t, this corresponds to an energy equivalent of 156 TWh.

The energy efficiency of technical electrolysers is between 70 and 80 %; the Sunfire company states efficiencies of up to 85 % for its systems [245].

On the basis of an electrolysis efficiency of 80 %, the electricity requirement for the production of hydrogen for the above-mentioned jet quantity is 195 TWh. It should be noted that only 1/3 of the hydrogen is chemically incorporated into the product. Two thirds are converted into water by the strongly exothermic synthesis reactions. Accordingly, the product contains only about 50% of the electrical energy used in chemically bound form.

For kerosene synthesis, the hydrogen demand can be estimated using the following stoichiometric equation:

Heating market

In 2015, final energy of 1,373 TWh was consumed in Germany for the provision of heating and cooling. At 669 TWh, the space heating market accounted for the largest share (see table below [246]).

Table 79 Final energy consumption for heating/cooling 2015 (D) in TWh [246]

	Total Heat	Space heat	Hot water	Process heat	Cooling
Electricity	177	16	21	84	56
Oil	205	169	21	15	1
Gas	586	313	49	223	1
Coal	126	9	0	117	0
District heating	119	64	9	45	0
Renewables (EE)	139	98	14	28	0
Other	21	0	0	21	0
Total	1.373	669	114	533	58
without electricity and EE	1.057	555	79	421	2

Broken down by final energy sources, electricity contributes 12.9% (177 TWh) and the direct use of renewables 10.1% (139 TWh) [246]. Deducting these energy quantities leaves a residual demand of about 1,050 TWh, which will have to be reduced in the future by increasing efficiency and ultimately covered by electrical energy in the course of sector coupling.

To estimate the electricity demand on the basis of today's heating and cooling demand, it is assumed that the energy demand for space heating and hot water can be provided by heat pumps. Assuming a coefficient of performance of 4, this would result in an electricity demand of 160 TWh. If the provision of process heat or cooling is taken into account, the total demand would add up to about 580 TWh.

For simplification, the inclusion of energy efficiencies for the conversion of final energy into heating/cooling was neglected, also against the background of greater uncertainties in the estimation of future demand.

It is expressly pointed out that the calculations and estimates presented were carried out solely with the aim of demonstrating the dimension of complete electrification in the course of sector coupling and greenhouse gas-free energy supply on the basis of current energy consumption. They cannot be used to show realistic future electricity requirements, as no reliable forecasts of demand development and technological progress are available.

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