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Gesellschaft für Chemische Technik
und Biotechnologie e.V.

TECHNOLOGY STUDY

Low carbon energy and feedstock for the European chemical industry

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The European Chemical Industry Council

Foreword

The chemical industry is an essential part of the modern societies we live in. By turning resources into valuable products and materials that enable many downstream value chains, the chemical industry delivers strong benefits and provides solutions to the grand societal challenges that the world needs to address in the 21st century.

The impact of CO_2 emissions is one of the most difficult challenges to be addressed. Virtually all human activities require energy and products that currently rely heavily on cheap and abundant fossil resources.

The chemical industry is no exception. It requires energy for running its processes, and feedstock - most often carbon feedstock, eventually embedded in most chemical products and materials - resulting in CO_2 emissions. However, the European chemical industry has a solid track record in reducing greenhouse gas emissions from its industrial operations. In addition, it delivers solutions to achieve major energy-savings in many value chains (e.g. construction with insulation materials, transportation with fuel-saving technologies and lightweight materials), with benefits in terms of CO_2 emission reductions.

The scope of this study is to analyse how the chemical industry could use breakthrough technologies to further reduce CO_2 emissions resulting from the production of its key building blocks. The purpose of this study is to provide quantitative data on promising low carbon technologies, estimate their potential impact on CO_2 emission reductions, and highlight the current technological and financial limitations and barriers.

Promising technologies are available at a relatively advanced stage of development, however their implementation on a wide scale is hard to achieve under the current framework conditions, while we also need to safeguard the benefits and the global competitiveness of this key industrial sector in Europe. This shows the need for a concerted approach between public and private stakeholders to further support an ambitious research and innovation agenda, with a strong focus on industrial relevance. It also shows the need, more than ever, for a close dialogue between public and private stakeholders about the regulatory framework that will allow the shift in the long run.

The study is a valuable input into the discussion on the future of the European chemical industry and the transition towards a carbon neutral society. Its key findings will hopefully foster a successful dialogue amongst key stakeholders.

Marco Mensink
Director General Cefic

Kurt Wagemann
Managing Director DECHEMA

Executive summary

In 2011, the European Commission published a 2050 energy strategy and roadmap with the ambition to reduce the GHG emissions in Europe by 80-95 % below the 1990 level. The Commission Energy Union Package issued in 2015 outlined the European vision as a sustainable, low-carbon and climate friendly economy. Such a political ambition requires a paradigm change supported by technological breakthroughs. This study sets out to understand the opportunities and challenges that the European chemical industry will face in the transition to carbon neutrality of its productions, including potential CO_2 emissions reduction, economic constraints, investments, research and innovation requirements.

The chemical industry and GHG emissions

The Chemical Industry is a solution provider for many downstream sectors and end consumer areas. The use of chemicals and materials (e.g. insulation materials, efficient lighting, lighter materials for transport, advanced materials for renewable technologies…) make substantial contributions to reducing energy demand and emissions across many sectors. A study compiling several life-cycle analyses (LCAs)[1] (2009) showed that for every unit of carbon it emitted in 2005, the industry's products enabled up to 2.6 units of CO_2-equivalent savings during the lifetime of those chemicals.

The European chemical industry is energy intensive. According to the study “Energy Efficiency Trends and Policies in Industry” (EC 2015), the chemical industry is the main industrial energy consumer with 19% of total industrial consumption. However, the industry has been able to decouple its energy consumption from its production, reducing its energy intensity by 56% since 1990; in parallel, the European chemical industry reduced its GHG emissions by 59%[2]. Today the chemical industry is the third largest GHG industrial emitter in Europe.

Technology options and Pathway scenarios to a 2050 carbon neutral chemical sector

Due to the diversity and complexity of the chemical sector a deliberate choice was made to focus this study on the main chemical building blocks used in upstream large volume production processes (i.e., ammonia, methanol, ethylene, propylene, chlorine and the aromatics benzene, toluene and xylene) that collectively represent two-thirds of the sector's current greenhouse gas (GHG) emissions. Their production through new low carbon processes is examined by considering further energy efficiency measures, the utilisation of

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[1] Innovations for Greenhouse Gas Reductions: A Life-Cycle Quantification of Carbon Abatement Solutions Enabled by the Chemical Industry, International Council of Chemical Associations, 2009, Amsterdam.

[2] Since 1990 the absolute primary energy consumption of the European chemical industry has been reduced by 22% and the GHG emissions by 59%, whilst the production of chemicals increased by 78% in the same timeframe.

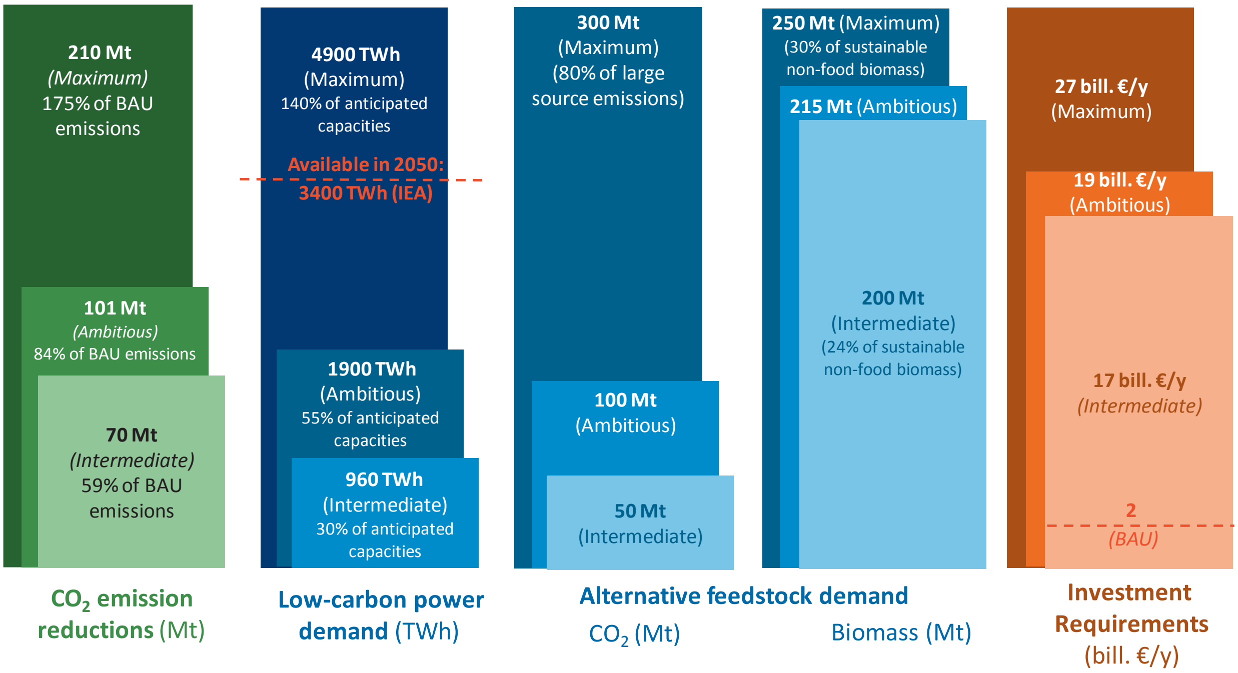
alternative carbon feedstock (i.e. bio-based raw materials and CO_2) and electricity-based processes that can benefit from a progressive decarbonisation of the power sector.

The penetration of these new technologies and processes is considered under 4 different scenarios with increasing levels of ambition, ranging from "business-as-usual" (BAU) (no deployment of low carbon options nor energy efficiency measures) up to "maximum" (theoretical potential with full implementation of low-carbon technologies including efficiency measures). For some products that can potentially be used as fuel alternatives (e.g. methanol, ethanol) the impact of leveraging the new low carbon technologies for the production of such alternative fuels has also been analysed.

Main findings - Barriers to achieving a carbon neutral chemical sector by 2050

The implementation of the technologies investigated in this study would allow for a very significant reduction of CO_2 emissions in 2050 (up to 210 Mt annually under the Maximum scenario). Including the production and use of fuels related to the pathways considered in this study, the additional CO_2 abatement potential in 2050 exceeds the chemical sector's current emissions even under the intermediate scenario.

However, such transition to carbon neutrality will entail huge challenges for the European chemical industry: availability of low carbon energy, availability of alternative feedstock, investments in new assets that far exceed the typical level of investments in the recent years, uncompetitive production costs.



Opportunities and challenges for various scenarios by 2050 (without fuels applications)

Some of the challenges are outside the control of the chemical industry. As an example, the transition will require access to abundant and cheap carbon-neutral energy that represents a very substantial part of, or could even exceed, the low-carbon power capacities anticipated by the IEA (International Energy Agency) in 2050.

Clearly, a main hurdle to overcome is the much higher production cost for the target building blocks addressed in this study if they were to be produced today with these low-carbon technologies. For instance, the production costs for ammonia, methanol, olefins and BTX (aromatics) would be two to five times higher than their fossil alternatives under current conditions. The issue of high feedstock cost (in the case of biomass) is further compounded by the relatively high cost of low carbon hydrogen for hydrogen based processes.

Recommendations

In order to achieve the EU's 2050 objectives, an ambitious Reaserch und Innovation (R&I) program will be essential to improve the potential of required advanced technologies, and public-private partnership efforts will be critical to enable fast deployment and risk sharing for the investments needed. In addition, industrial symbiosis opportunities and sustainable materials recycling options should be further explored in order to improve energy and resource efficiency beyond sectorial boundaries.

Nevertheless, innovation alone cannot close the huge gap in production costs highlighted in this study. Enabling a path to carbon-neutrality will require an intense dialogue between public and private stakeholders for all parties to understand the size of the challenges and the implications, taking into account the global competitiveness of the European chemical industry.

The findings of this study can support a fact based discussion on challenges and opportunities for the European chemical sector in this process.

Technical Summary

The objective of this study is to explore options towards a carbon-neutral European chemical industry. This entails the description of pathways for a transition of production processes towards low-carbon production, by further exploiting energy and resource efficiency measures, increasingly by using alternative carbon feedstocks i.e. renewable raw materials (biomass) and CO_2, which can replace fossil feedstocks and leverage a lower overall carbon footprint, and by exploring possibilities to use electricity-based processes that can benefit from a progressive decarbonisation of the power sector. The diversity and complexity of the chemical industry makes it impossible to cover all aspects, processes and products. It was therefore a deliberate choice at the beginning of the study to focus on the main chemical building blocks that are upstream of many processes and that represent large production volumes with a significant fraction of today's industry GHG emissions: ammonia and urea, methanol, ethylene, propylene, chlorine and the aromatics benzene, toluene and xylene. Apart from the description and assessment of the major low-carbon process routes, synergies and opportunities of industrial symbiosis with other process industries are explored, in which the chemical industry can valorise side streams and waste from these other sectors. Likewise, the impact of recycling of polymers and polymer waste as feedstock is considered.

As a separate element, the study also investigates the implications of producing synthetic fuels as a potential contribution of the chemical industry to decarbonisation of the transport sector.

The study describes technical options and challenges as well as economic constraints, necessary investments, research and innovation needs and framework conditions that have to be in place to deploy the described technical options. The potential impacts are described on the basis of four deployment scenarios with different ambition levels:

- **business-as-usual (BAU)**, assuming no implementation of new technology options and no further advancement of efficiency measures,
- i**ntermediate, (Interm)** describing a moderate level of ambition and slow but continuous deployment of low-carbon technologies,
- **ambitious (Amb),** depicting a high level of ambition and strong support of all stakeholders to overcome any constraints,
- **maximum (Max),** describing the theoretical potential, i.e. upper limit of possible CO_2 reductions.

As a basis of the scenario work, the IEA 450 ppm scenario and the IEA ETP2015 2°C model have been used to consider e.g. the future energy mix and fuel demand. Furthermore, a 1 % growth per annum is assumed for the EU chemical industry.

CO_2 emission reduction potentials

Implementation of the technologies investigated in this study allow for a reduction of CO_2 emissions up to 210 Mt annually (max) in 2050. In the considered range of ambitions, between

70 Mt (Interm) and 101 Mt (Amb) CO_2 can be mitigated, corresponding to 59% to 84% of the anticipated emissions in 2050.
20 to 30 Mt CO_2 of these emission savings can be achieved by further efficiency measures and plant retrofits, transition to a power-based heat and steam generation and recuperation of waste heat. The main share of the additional savings is enabled by chemical production of ammonia using hydrogen from low-carbon electricity and production of methanol, olefins and BTX from hydrogen and carbon dioxide. These processes benefit from avoided fossil emissions and a considerable amount of carbon from CO_2 built into the products, thereby enabling a CO_2 recycling and avoidance of fossil feedstocks. Hydrogen based ammonia with 1.7 t and methanol with 1.5 t avoided CO_2 per ton of product are particularly efficient in this respect. Chlorine production as already existing electrolysis based process will benefit from a progressive decarbonisation of the power sector without the need for a new process pathway. The biomass based production of the petrochemical building blocks targeted in this study entails multiple steps and a relatively inefficient use of biomass, demanding high amounts of biomass, at the same time enabling only limited CO_2 avoidance potential. In fact, production of BTX from biomass shows even higher process related GHG emissions compared to the established fossil pathways. Rather than producing drop-in petrochemicals from biomass it is recommended to exploit more efficient synthesis of target products that maintain the functional units of the feedstock molecules, e.g. oxygen-rich and carbonated molecules such as polylactic acid and succinic acid.

If the production of fuels is added to chemical production in the scenarios, the CO_2 abatement potential in 2050 increases to 117 Mt in the Interm and 216 Mt CO_2 in the Amb scenario, corresponding to 98% - 180% of the chemical sector's own emissions projected in 2050. As fuels, methanol as gasoline additive, bioethanol and synthetic diesel and jetfuel produced from hydrogen via Fischer-Tropsch synthesis have been considered. Main impact is delivered by the low well-to-wheel footprint of the synthetic drop-in fuels compared to the fossil equivalents.

For industrial symbiosis, collaboration with the steel industry seems particularly promising, as the off-gases of steel manufacturing contain high amounts of carbon monoxide but also hydrogen that can be valorized as syngas. The amount in Europe would suffice to supply the production of 55 Mt methanol.

Recycling of polymers and the use of polymer waste as feedstock for chemical processes would leverage large energy saving potentials. Comparing the energy demand of polymer recycling from a study by Accenture[3] with the energy demand of de novo synthesis in this

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[3] Accenture, Taking the European Chemical Industry into the Circular Economy, https://www.accenture.com/us-en/insight-circular-economy-european-chemical-industry

study suggests cumulated potential energy savings up to 57 Mtoe by 2050, which is more than the fuel and power consumption of the EU chemical industry of one year. Quantification of the CO_2 emission reduction would require a detailed analysis of the carbon footprint of recycling routes considering energy required, properties and added value of recycled polymers vs. de novo products.

Reaching CO_2 emission reductions for the chemical industry by 2050 in the range quantified above would entail:

- a demand in *low carbon power* that considerably exceeds the amount of such low carbon power predicted by the IEA to be available in Europe by 2050; The demand ranges from 960 TWh (30% of the projected available supply) in the interm via 1900 TWh (55%) in the Amb scenario to 4900 TWh (140%) as maximum potential for chemical production. If fuels are included the demand increases to 2000 TWh (60%) 4600 (135%) a11700 TWh (350%) respectively.
- a demand for CO_2 as feedstock in the range of 50 (Interm) to 300 Mt (max) for chemicals and 110 to 670 Mt for chemicals and fuels; The IEA expects 380 Mt from large stationary sources, which would be sufficient to cover the Interm and Amb scenario but would run short for the maximum potential, if fuels are included.
- a demand for biomass as feedstock ranging from 200 to 250 Mt is required under the investigated scenarios. This roughly corresponds to 30% of available sustainably produced non-food and feed biomass (i.e. lignocellulosic and waste biomass) in Europe. Further extension of the ambitions would therefore be prohibitive.
- A demand for extensive additional investments; based on investment costs of 2,1 billion € per annum for the reference scenario, 14,1 billion € for implementing efficiency measures, and 17,0, 19,2 and 26,7 billion € per annum for the Interm, Amb and Max scenarios would be required respectively. Since the processes under consideration only represent a part of the chemical industry, the most energy intensive, but not necessarily the most invested-in part, this would amount to a significant additional investment on behalf of Europe's chemical industry, which is already in tight global competition.

For the chemical industry, the transition to carbon neutrality will entail *enormous* challenges, some of which are usually not under control of the chemical industry. The transition will require access to abundant and cheap carbon-neutral energy. Carbon-neutrality of the chemical sector therefore relies on a much more ambitious extension of low-carbon power capacities, at least a factor 2 of the level currently anticipated by the IEA, to meet its needs. The chemical sector then would probably demand the output of this additional 100% capacity extension.
Feedstocks, including biomass and process gases such as CO_2 and CO need to be available at low prices, competitive if not lower than fossil feedstocks in the long term. Very large investments are required and major changes in the current assets are foreseen.

A main hurdle to overcome is the relatively high production cost of the target building blocks in case of the low-carbon technologies. While power-based steam generation and heat recuperation by steam recompression are technologies that already seem competitive in terms of costs, the production costs for ammonia, methanol, olefins and BTX are currently 2-5 times higher than the fossil alternatives. This is related to high feedstock cost (in the case of biomass) and high cost of electricity (in the case of hydrogen based processes). For electrolysis based processes it has to be pointed out, that the economic gap is partly intrinsically, as the generation of chemical building blocks from water and CO_2 is obviously more energy, resource and cost-intensive than using existing fossil energy carriers.

For some of the essential building blocks, the suggested process pathways are not very efficient and the development of alternative processes is required. This is particularly the case for BTX production from biomass, for which no mature technology is available.

Based on these findings, the following key actions are recommended:

- Realisation of a large and ambitious R&I program to further investigate the potential of new technologies, including low-carbon hydrogen production, CO_2 utilisation, lignocellulosic biomass use for chemical and biochemical synthesis and advanced concepts for waste heat recovery;
- Public-Private-Partnerships (PPPs) to focus RD&I efforts and to enable risk sharing for investments for demonstration of innovative technologies; fast realization of demonstration plants at scales beyond 5kt/a with lighthouse character are a prerequisite;
- Enhanced cross-sectorial collaboration and exploration of industrial symbiosis opportunities creating synergies and improving energy and resource efficiency beyond sectorial boundaries;
- A dialogue with policy makers to point out the barriers and constraints and to facilitate market-uptake.
- Generation of a central European database of CO_2 sources and infrastructures that would provide potential for industrial symbiosis, including e.g. emitters below the threshold for reporting to the European Pollutant Release and Transfer Register; likewise, a database on the available sustainable biomass and a central database for lifecycle data.

In terms of R&I priorities a strong focus has to be provided on technologies for hydrogen generation, as hydrogen is a key enabler for a major part of low-carbon technologies. This includes improvements in system lifetime and performance as well as scale-up of stacks. The less mature technologies have to be developed further - in particular Solid Oxide Electrolysis provides high potential advantages in efficiency and in the long term also cost benefits. Power-to-Heat technologies (electrical heat pumps) should be further developed to extend operating window to temperatures > 250 °C. For biomass, selective pyrolysis (catalytic fast pyrolysis) of lignocellulosic biomass or hydrogenation of lignin to depolymerize the complex lignin structure and stabilize reactive intermediates are important R&I priorities providing access to aromatic compounds. CO_2 utilisation in general is an emerging field with remarkable progress within the last 5 years. Direct electrocatalytic conversion to e.g. produce ethylene directly from CO_2 is an interesting option. Photocatalytic processes are still in a fundamental stage, but should be further investigated.

Nevertheless, further innovation only is not expected to close the gap in term of production costs. Hence a change of framework conditions is necessary as part of a joint effort with public stakeholders if we embark *together* in the direction of carbon-neutrality while ensuring the global competitiveness of the European chemical industry. A dialogue is vital for relevant private and public stakeholders to understand the size of the challenges and implications.

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List of abbreviations

%	Percent
€	Euro
ASU	Air Separation Unit
BF	Blast Furnace
BOF	Basic Oxygen Furnace
BPT	Best Practice Technology
CAPEX	Capital expenditure
CCS	Carbon capture and storage
CCU	Carbon capture and utilisation
CP	Coke plant
CRI	Carbon Recycling International
CSP	Concentrated solar power
DEA	Diethanolamine
DME	Dimethyl ether
EC	European Commission
EJ	Exajoule
EtL	Emission to Liquid
ETP	European Technology Platform
ETS	Emission Trading System
EU	European Union
FAME	Fatty Acid Methyl Esters
FQD	Fuel Quality Directive
g	Gram
GHG	Greenhouse gas(es)
GJ	Gigajoule
GW	Gigawatt
h	hour
IEA	International Energy Agency
K	Kelvin
kJ	Kilojoule
kWh	Kilowatt hours
LNG	Liquefied natural gas
m^3	Cubic meter
MDEA	Methyldiethanolamine
MEA	Monoethanolamine
mill.	Million
MJ	Megajoule
mol	mole
MTBE	methyl-tert-butyl ether
MTG	Methanol-to-gasoline
MTO	Methanol to olefins
MTP	Methanol to propylene
MW	Megawatt
MWh_{el}	Megawatt hours of electrical power
NG	Natural gas
Nm^3	Norm cubic meter (volume at 0°C, 1 atm)
No	Number
Pa	Pascal
PEM	Proton exchange membrane
PJ	Petajoule
ppm	Parts per million
PtX	Power to X (e.g. gas, liquid, fuels)
pX	p-Xylene
RD&I	Research, Development and Innovation
RED	Renewable Energy Directive
REN H_2	H_2 produced with renewable energy
RWGS	Reverse water gas shift
SEC	Specific Energy Consumption
SNG	Synthetic natural gas
SOE	Solid-oxide electrolysis
SRM	Steam reforming of methane
T	tons
Toe	tons of oil equivalent
T	Temperature
TAME	Tertiary amyl methyl ether
TRL	Technology readiness level
tpd	Tons per day
TWh	Terawatt hours
VAT	Value added tax
ΔH^0	Standard enthalpy of reaction

1 Introduction

1.1 Background

The chemical industry is an energy intensive industry. In 2014, the fuel and power consumption of the EU chemical industry including pharmaceuticals, amounted to 52.6 Mtoe (2.2 EJ or 612 TWh)[4], 19.5% of the overall EU industrial energy consumption. Corresponding process related CO_2 emissions of the chemical industry have been at 120 Mt in 2014. Continuous efforts in terms of energy efficiency measures have already resulted in a decrease of total greenhouse gas emissions by 59% compared to the 1990 level, despite an expanded production of 78%, showing a decoupling of production vs. emissions. However, this decoupling has limitations, and the major part of efficiency gains has already been leveraged, at least for the large scale chemical products.

In terms of CO_2 emissions, the downstream use of chemicals such as insulation materials, efficient lighting, lighter materials for automobiles and advanced materials for renewable technologies has to be taken into account. These chemical products make substantial contributions to reducing energy demand and emissions across many sectors. A study compiling several life-cycle analyses (LCAs) showed that for every unit of carbon it emitted in 2005, the industry's products and technologies enabled 2.1 to 2.6 units of CO_2-equivalent savings (compared to non-chemical alternatives)[5].

The EU 2050 package aims at getting closer to a carbon-neutral economy. The low-carbon economy roadmap suggests that the EU should cut greenhouse gas emissions to 80 - 95% below 1990 levels by 2050. Envisioned milestones to achieve this are 40% emissions cuts by 2030 (EU 2030 Energy and Climate Policies communication) and 60% by 2040. This political ambition needs to be translated into real technology breakthroughs that will enable the transition towards carbon neutrality.

For the chemical industry "decarbonization" is intrinsically impossible, as a major part of the chemical industry is carbon based, meaning that carbon feedstocks are required as raw materials to manufacture the large range of products to supply virtually all downstream sectors, from rubber and plastics, construction, automotive, pulp and paper, textiles to agriculture. Today, fossil feedstocks are the predominant source of carbon for the chemical industry. From 78.6 Mt of feedstocks in the EU chemical industry, 73% are based on mineral oil, 16% on natural gas, 1% on coal and 10% (8 Mt) on renewable feedstocks (biomass).

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[4] European Chemical Industry Facts and Figures Report 2016, Cefic; http://www.cefic.org/Facts-and-Figures/

[5] Innovations for Greenhouse Gas Reductions: A Life-Cycle Quantification of Carbon Abatement Solutions Enabled by the Chemical Industry, International Council of Chemical Associations, 2009, Amsterdam.

The demand for chemical products will further increase in the future, and hence the chemical industries' demand for carbon-based feedstock. CO_2 emissions from the chemical industry could then increase as soon as resource and energy efficiency potentials have been exploited.
In light of international climate protection targets and the EU ambitions, the chemical industry needs to explore its contributions to the goals of a carbon-neutral economy, what the envisioned targets mean for the sector and what the necessary transition entails from a technology point of view, in summary: "What does it entail for the chemical industry to be carbon-neutral by 2050?"

1.2 Scope of the study

The objective of this study is to explore options for a low-carbon European chemical industry. This entails the transition of production processes towards low-carbon production, by further exploiting energy and resource efficiency measures and increasingly by replacing fossil feedstocks by alternative carbon feedstocks leading to a lower CO_2 footprint.
The study provides a forward-looking comparative overview of technology options with their limitations and elements of technical feasibility and economic viability assessment. The study further provides a set of scenarios on how to achieve the defined emission reduction targets by combining and deploying the analysed technologies including potential transition phases with bridging technologies. The time horizon for the scenarios and the enabling technologies considered is 2050, to be consistent with the envisioned time frame of the EU 2050 strategy.
The chemical industry is not operating in an isolated framework. Contributions from other sectors, in particular the energy sector, are necessary to achieve emission reductions for the chemical industry. Corresponding requirements and necessary framework conditions are therefore included in the study. Likewise, synergies with other process industry sectors in terms of industrial symbiosis are considered.
The impact of chemical products on downstream emissions is not within the scope of this study and has not been assessed. However, as only exception, the possible implications of the chemical industry providing synthetic non-fossil fuels for the transport sector have been investigated, as i) in some cases the same chemical products can serve as both chemical raw material and transport fuel (methanol, SNG), and ii) process technologies described in this study can be used to synthesize high quality synthetic fuels (e.g. Power-to-X technology).

1.2.1 Products included in the study

Production pathways in the chemical industry are complex; hundreds of different chemical processes are used to manufacture thousands of chemicals, intermediates and polymers. In order to limit complexity, this study focuses on the production of the 9 largest petrochemical/chemical products in Europe in terms of production volumes, which account for more than 50% of the chemical sector's energy demand and CO_2 emissions.[6] More important, these 9 products are the essential building blocks of virtually all organic chemical products in the current petrochemical value chains.

The study quantifies emission reduction potentials of low carbon production technologies for the following high volume petrochemical/chemical products in Europe:

- Methanol
- Ethylene and propylene
- Benzene, toluene, xylenes (BTX)
- Ammonia and urea
- Chlorine

For the production of synthetic fuels for the transport sector, the product range is extended to cover the following products:

- the production of methanol as substitute and/or additive in gasoline
- the production of bioethanol as gasoline additive
- the production of synthetic diesel as drop-in fuel
- the production of synthetic kerosene as drop-in jetfuel.

Apart from these products, several chapters mention process routes yielding other chemical products, if such routes provide particular benefits that are worth mentioning in the context of a low-carbon chemical industry.

1.2.2 Technology options investigated

The study investigates a broad portfolio of technologies that potentially contribute to the chemical sector's emission reduction. In a nutshell, three aspects are combined in the analysis: i) improvement of energy efficiency in conventional production plants, ii) transition of the feedstock base towards alternative carbon sources, i.e. CO_2 originating from various industrial point sources, biomass as a renewable feedstock and carbon-containing products reused in recycling processes, and finally the use of low-carbon electricity (renewable electricity and nuclear power) for energy supply (and electrons as reducing agent) in chemical transformations. The investigated options are described subsequently. As the anticipated timeframe is 2017 - 2050, and technology implementation from investment decision to start of operation is usually in the order of 10 years, the focus of this study is on technologies, which

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[6] Technology Roadmap "Energy and GHG Reductions in the Chemical Industry via Catalytic Processes; IEA/ICCA DECHEMA, 2013.

are at least proven and demonstrated on pilot plant scale, i.e. available at technology readiness levels (TRL) 6 and higher. Low TRL technologies, i.e. technologies at TRL2-4 investigated in fundamental and lab research activities are not considered to constitute a commercial production pathway by 2050 and to contribute to real emission reduction within the envisioned timeframe. Nevertheless individual pilot or demonstration activities might emerge for some technologies at TRL 4-5 and are discussed. Corresponding technologies at very low TRL are for example artificial photosynthesis or biotechnological CO_2 conversion routes including approaches like microbial electrosynthesis.

1. Energy efficiency: This option relates to estimates on **energy efficiency potentials** that can be leveraged to reduce the GHG intensity of the chemical industry in Europe. Efficiency gains are a mix of continuous retrofits of existing plants to reduce the specific energy consumption (usually incremental improvements) and replacement of old plants/building of new plants thereby using the available technologies that represent the best performing plants.

2. Hydrogen and CO_2 based production routes: These pathways entail the use of low-carbon electricity to produce hydrogen and subsequent reaction of the hydrogen with carbon dioxide from industrial installations to produce chemicals and fuels. These routes are often referred to as Power-to-Chemicals, Power-to-Gas/Liquids or Power-to-X. Within the scope of this study a) reforming of CO_2 to deliver methanol, either directly or via syngas, with subsequent methanol value chains or b) using the formed syngas to produce hydrocarbons via Fischer-Tropsch synthesis are considered. CO_2 resulting from many industrial processes and fossil-fired power plants serves as a carbon source here and is re-introduced in an industrial carbon-cycle via these pathways. In the case of synthetic fuels from CO_2 and hydrogen, well to wheel emissions are compared to the corresponding fossil fuels to quantify the emission reductions.

3. Biomass and biomass waste streams to chemicals: This pathway includes the use of biomass, in particular lignocellulosic biomass and waste streams to produce chemicals either via a) chemical or biotechnological conversion of biomass or b) biomass gasification and subsequent conventional syngas-based chemical routes. Emission reduction is enabled via the substitution of fossil feedstock by biomass with correspondingly lower carbon footprint.

4. Electricity-based processes: In addition to the already described Power-to-X technologies, low-carbon electricity can be used for steam generation in electric boilers replacing natural gas fired boilers (Power-to-Heat). This route is already considered or even operated by large chemical producers, because it can be flexibly employed as demand-side management measure to use low-cost intermittent power supply from renewables. Due to the substitution of natural gas it constitutes a low-carbon measure. As a second route, steam recompression, i.e. compression of low temperature low pressure steam before condensation is considered.

Another process included under this point is chlorine production, which is already a 100% electricity-based process.

5. Industrial symbiosis and circular economy

The technology options described under 2. demand large amounts of hydrogen as well as carbon dioxide as feedstock. As syngas routes play an important role, sources of carbon monoxide are also important to consider. The study therefore describes elements of industrial symbiosis with other process industries (steel, cement) and the power sector, in which the chemical industry could valorise waste streams of H_2, CO_2 and CO from these other sectors. Other potential industrial symbiosis opportunities such as cross-sectorial heat integration have not been taken into account, as these contributions substantially increase complexity and mutual dependency of production sites across sectors.

As part of the concept of circular economy, the impact of recycling of polymers and polymer wastes as feedstock is considered. The use of these "secondary raw materials" can be less energy-demanding than the de novo synthesis and reduces the amount of primary feedstocks. Assessment of the CO_2 emission reduction potential would require detailed LCA of recycling routes.

6. Other technologies: Apart from technology options summarized under 2., a number of **CO_2 utilisation routes not requiring hydrogen as direct reactant** are currently developed. Major routes are i) copolymerization with CO_2 as building block and ii) synthesis of various chemicals from CO_2, including acrylic acid, cyclic carbonates, aldehydes etc. These routes will be briefly described but not included in the scenario work as the corresponding products are not covered by the studies' scope.

Carbon capture and storage (CCS) is a general pathway for decarbonizing large production sites. The Cefic roadmap "European chemistry for growth" identified ammonia, crackers and combustion in general as potential sources. However, in light of the anticipated CO_2 utilisation scenarios, in a phase of advanced technology deployment, the chemical industry will evolve as net importer of CO_2 to supply the demand of CO_2 as feedstock. CCS as technology path in this respect is considered counterproductive at this point. As such usage is regarded as the preferential pathway over storage.

Capture and purification of CO_2 to supply the described chemical processes in this study are a prerequisite. Capture technologies are available and are a field of intense research activities, including purification technologies tailored to specific conversion routes, this study therefore does not describe capture technologies in detail. An exception is **direct air capture** of CO_2, which is discussed as an option that might get relevant in future, if the availability of industrial CO_2 sources decreases due to the wide implementation of low carbon technologies in these sectors.

1.2.3 Scenario work in this study

In terms of quantitative CO_2 reduction potentials, scenarios have been developed, which describe the corridor of possible impact. The current status of CO_2 emissions in the production of the above listed chemicals form the basis in a **business-as-usual scenario (BAU)**, assuming no implementation of new technology options and no further advancement of efficiency measures. It should be pointed out that the assumed "freeze" in technical advances and energy efficiency improvements in the BAU scenario does not reflect the reality with steady incremental technological improvement that is common practice in the chemical industry. It has been chosen to quantify the impact of all combined technology measures described in this study in comparison to *today's* energy intensity and CO_2 emission level (baseline).

The **maximum scenario (Max)** describes the theoretical potential, i.e. the upper limit of possible CO_2 reductions by complete implementation of the described technologies in the European chemical industry and potential impact on the fuel sector by 2050.

In between these lower and upper boundaries, two scenarios are considered:
The i**ntermediate scenario (Interm)** assumes continuous improvements of process efficiencies by efficiency measures and a slow starting, but steadily increasing deployment of breakthrough technologies. It is further assumed that policy measures are taken to support low-carbon breakthrough technologies and that pathways become sufficiently competitive in order to replace fossil routes. The intermediate scenario already includes a substantial replacement rate of existing older plant capacities, and therefore represents a relatively high level of ambition compared to the BAU scenario.

The **Ambitious (Amb)** scenario is considered as very ambitious and is only feasible with full support of all stakeholders and under most favorable framework conditions, disregarding economic constraints. It is based on the consequent implementation of technology options, a fuel sector fully supporting the transition to carbon-neutral fuels, immediate start and minimum time for R&D, pilot or demonstration activities, as well as commercial deployment without delays. Full policy support is provided and no economic constraints hamper the implementation. A considerable share of old, fully depreciated plants is replaced early.

1.3 Basic assumptions and data used

The development of scenarios requires a number of basic assumptions and data as basis. The following assumptions have been made:

- The IEA 450 ppm scenario is assumed in 2050 for the primary energy mix (as outlined in the World Energy Outlook 2015). Low-carbon (nuclear, renewable) is anticipated to evolve and be available between now and 2050 as foreseen in the 2°C scenario of the IEA

European Technology Perspective (IEA-ETP) 2015 documents. The IEA-ETP model is largely consistent with the model used for the World Energy Outlook (WEO). Data from the ETP2015 model have used very consequently in this study to ensure the maximum consistency. This includes e.g. energy supply and gross electricity generation with breakdown into primary energy sources in Europe, fuel demand and breakdown to fuel types, the evolvement of the carbon footprint of the electricity mix, and direct CO_2 emissions of industry and the power sector. It has to be emphasized that these IEA data sets do not necessarily reflect the future, and are as such based on a scenario. The used 2°C scenario (2DS) already includes ambitious targets and measures for emission reduction.

- The European chemical industry is expected to continue to deliver substantially the products and materials required by society. A 1 % growth per annum is assumed for the EU chemical industry including the petrochemicals investigated in this study. Regional changes in chemicals production, shift of production to other world regions outside Europe and potential carbon leakage effects are not considered in the scope of the study.
- Current production volumes in Europe have been taken from IEA/IHS data as well as prodcom[7], Eurochlor[8] and Fertilizers Europe[9].
- The production of fuels and corresponding decarbonisation potentials are included in the study, otherwise “handprint”, i.e. the impact of chemical products on CO_2 emission reduction of downstream sectors is out of scope.

In addition to the basic assumptions, the evaluation of the different technologies and the subsequent impact scenarios rely on a large number of additional technical and economic assumptions and assumptions on the rate of technology implementation. These are described in the respective chapters. For critical parameters a sensitivity analysis is provided to show the impact of assumptions. However, scenarios are provided with <u>one</u> consistent set of assumptions to avoid a higher level of complexity.

1.4 Definitions

Unless stated otherwise, energy consumption of a process is usually referred to as **specific energy consumption** (SEC), which is amount of energy, expressed in GJ/t, that an average plant requires to produce a specific product. The SEC includes net electricity and fuel consumption to provide heat, hence processes generating electricity or supplying excess steam are accounted for in the SEC.

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[7] http://ec.europa.eu/eurostat/web/prodcom
[8] Euro Chlor Industry Review 2015-2016; http://www.eurochlor.org/media/106905/euro_chlor_review_web.pdf
[9] Fertilizers Europe Industry facts and figures 2015; http://fertilizerseurope.com/index.php?id=14

The **total energy demand** in addition to the SEC contributions also includes the energy required to produce the feedstock used in the process and the energy content of the feedstock which is built in the product.

Throughout the study, processes based on low carbon technologies are compared with conventional fossil based processes. The study therefore often refers to the terms **additional energy demand** and **additional electricity demand**, meaning the difference in energy or electricity demand of the low-carbon process compared to the fossil reference process.

Electricity use in the low-carbon processes described in this study usually means low-carbon electricity from renewable sources (or nuclear power). The carbon footprint of low-carbon electricity is not set as zero, as for instance the building of a wind power plant and electricity production and transport causes CO_2 emissions. This is accounted for in the study by using appropriate LCA values. In the various scenarios, low-carbon electricity needs are quantified and compared to planned low-carbon power production capacities.

The **carbon footprint** of processes is compared based on a uniform set of assumptions. Emissions during synthesis of the target product comprise energy related emissions (i.e. heat and electricity) and process related emissions (e.g. CO_2 generated in ammonia synthesis). Energy related emissions are completely allocated to the chemical industry, this includes the carbon footprint allocated to the supply of the power required for electricity based processes. This is different from the usual sector allocation, where the carbon footprint of electricity would be allocated to the power sector. In this sense, cradle to gate contributions to the carbon footprint are generally used, unless stated otherwise. For instance, production of methanol from natural gas includes the production and supply of natural gas and the process chain of steam reforming and methanol synthesis. Production of methanol from hydrogen and CO_2 includes the supply of electricity for electrolysis of water to produce hydrogen, the electrolysis process itself, capture and supply of CO_2 and subsequent methanol synthesis.

A special approach has been chosen to account for the CO_2-based carbon incorporated into the product. From an LCA perspective, the ISO/TS 14067[10] would demand a separate and different accounting of biogenic and fossil carbon. In case the CO_2 used as carbon source is extracted from the atmosphere via a biological system (biomass growth) or a technical system (air capture), it would count as negative emission at the beginning of the product lifecycle and would be emitted again at the end of the product's life, yielding an even CO_2 balance. CO_2 from power plants or industrial processes however represents fossil-based CO_2 and would be counted as emission at the beginning of the product lifecycle. This common LCA practise disregards the concept of CO_2 recycling which is assumed in this study. CO_2 utilisation in this

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[10] ISO/TS 14067: 2013 Greenhouse gases -- Carbon footprint of products -- Requirements and guidelines for quantification and communication

sense represents a recycling of carbon, in which recycled CO_2-based carbon substitutes a corresponding amount of fossil carbon, which would otherwise be required as feedstock and which would add further CO_2 to the GHG inventory of the atmosphere at the end of the product life. CO_2-based carbon incorporated into the product has therefore been counted as negative emission throughout the study, irrespective of the origin of the CO_2 (biogenic or fossil). It has to be pointed out that the concept of CO_2 recycling is only valid, as long as CO_2 from fossil sources occurs as an unavoidable and undesired by-product of power supply or industrial production. Generating CO_2 deliberately and with the only motivation to supply it as carbon feedstock for chemical production would not fall into the category of recycling, and the corresponding CO_2 would definitely have to be counted as emission. For the example of CO_2-based methanol synthesis, 1.373 t of CO_2 are stoichiometrically built in the product, which would be counted as negative emission. The same approach of negative emission accounting has been used for biogenic carbon built in the product.

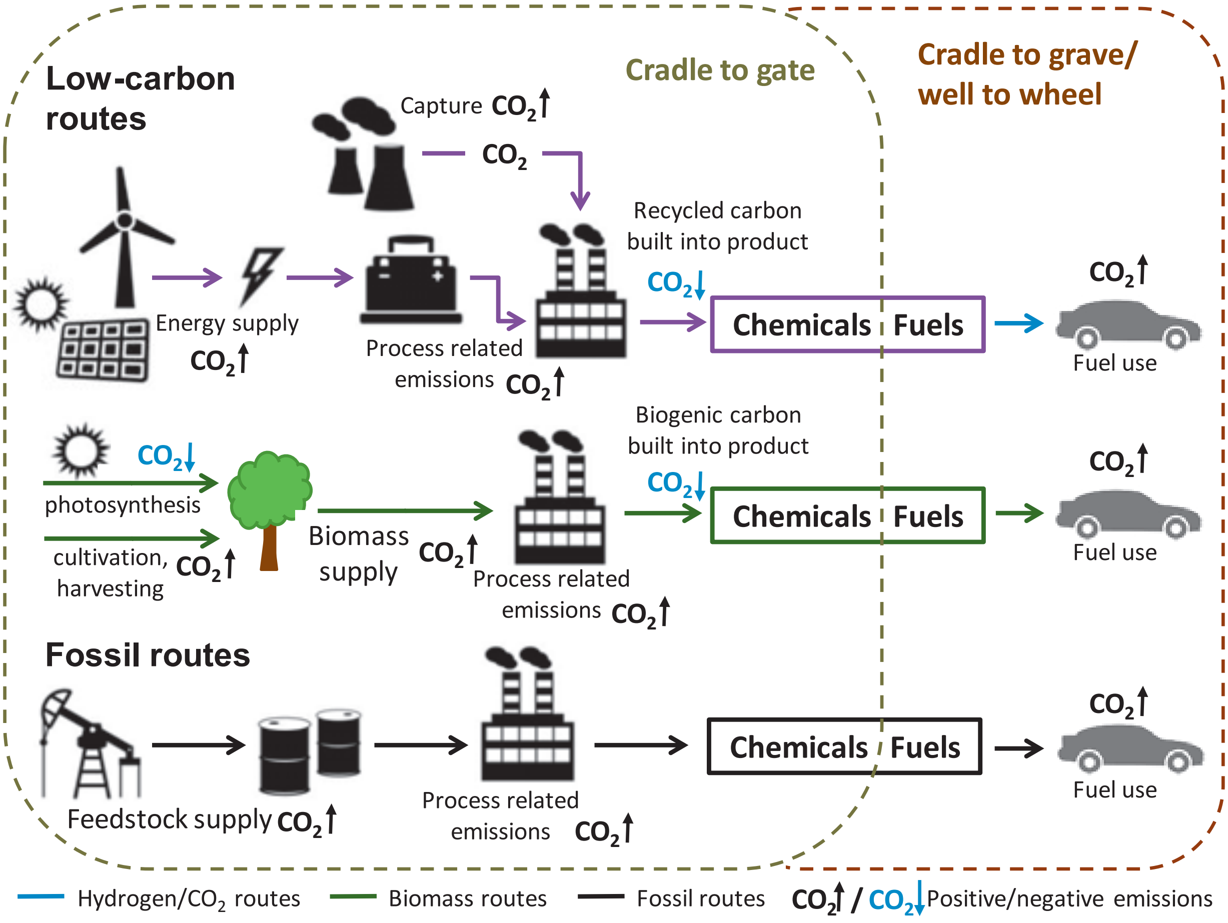

Figure 1: Contributions to the carbon footprint for different process routes and system boundaries for chemicals vs. fuels; for fossil routes, energy supply is included in the feedstock

The product use phase is not considered, with the exception of transport fuels, as the impact of synthetic fuels on the transport sector has been explicitly included in the scope of the study. The carbon footprints of transportation fuels are therefore based on well-to-wheel emissions, i.e. including combustion of the fuels. Figure 1 schematically summarizes the various contributions described in this section.

Avoided CO_2 is a frequently used measure in this study. It refers to the difference of the carbon footprint of the low-carbon process compared to the fossil reference process. All contributions to carbon footprint depicted in Figure 1 are included for both the low-carbon and the fossil process. In the comparison of technologies, avoided CO_2 is expressed as ton CO_2 per ton of product. In the scenarios, this figure is multiplied by the production volume to calculate the potential of CO_2 emission reductions based on the implementation of the low-carbon process alternative. In the case of the transportation fuels, the avoided CO_2 furthermore includes the emissions in the use phase and therefore covers well-to-wheel emissions.

2 Energy efficiency potentials

Since 1990, the European chemical industry has put tremendous effort into the improvement of energy efficiency and hence decoupling of production from energy consumption and greenhouse gas emissions. Despite increasing production volumes by 78% between 1990 and 2014, fuel and power consumption fell by 22% from 67.5 to 52.6 Mtoe, greenhouse gas emissions fell by 59.4% from 324.5 to 131.6 Mt in this time period.[4] The relatively stronger emission reductions are a result of shifting towards less carbon intensive fuels and reducing process emissions including for instance N_2O abatement in nitric acid plants.

Further measures to reduce the carbon-intensity of the currently used petrochemical processes via efficiency measures may include

- Incremental improvements,
- Implementation of best practice technologies, i.e. production with plants at the highest available energy efficiency level
- advanced heat integration
- further advancements such as the use if process intensifying equipment

2.1 Incremental improvements

Incremental improvements refer to small and anticipated technological advances in the "normal course of business". Examples include more selective, active and/or durable catalyst systems, optimised reactor performance, higher levels of heat integration, improved operating conditions, etc. Many such improvements are retrofits to already existing plants. Data received from a survey of chemical manufacturers and feedback from other industrial experts done by DECHEMA in the course of the IEA/ICCA/DECHEMA Technology Roadmap in 2013[6] indicates, that incremental improvements for specific processes can yield improvement (i.e. cause a decrease) of energy intensity in the range of 0.2% to 1% per year.

2.2 Implementation of best practice technologies

Best practice technologies (BPT) refers to widespread deployment of best practice/established technologies in existing plants or new facilities. Average European production plants have undergone a series of retrofits during their lifecycle and are operating at a high level of energy efficiency, but the SEC is usually above the level of BPT. Table 1 lists SEC and BPT levels for several processes relevant to this study.

BPT efficiency level usually cannot be achieved via retrofits of old plants and is therefore only relevant for new installations. In the scenario work of this study, the extension of production capacities with the assumed 1% growth rate of the chemical production in Europe (see chapter 1.3) and the necessary replacement of old installations is predominately reserved to the new low-carbon technologies to meet the ambitions of the different scenarios. An exception is chlorine for which production will continue to be based on conventional technologies.

Table 1: Average Specific Energy Consumption and Specific Energy Consumption of best practice technologie

Process	Actual SEC (unit)	OECD Europe	World average	BPT
Naphtha-based steam cracking	GJ/t HVC	12.2	13.8	12.0
Natural gas-based methanol	GJ/t methanol	12.5	13.8	9.8
Natural gas-based ammonia	GJ/t ammonia	16.6	17.8	9.0

2.3 Advanced heat integration

SPIRE estimated 20–50% of the energy used in industrial processes to be lost as hot exhaust gases, cooling water and heat losses from equipment and products[11]. For the large petrochemical processes, a high level of heat integration on plant and site level has usually been achieved in Europe, deficits exist more for smaller, isolated installations, and low-to medium production processes, which are often realized in batch processes. Further optimisation of heat integration and heat cascading can further reduce the energy use. In a recent study, Ecofys points out heat pumps, heat-absorption and cooling and Organic Rankine Cycles as advanced technical solutions.[12] Furthermore cross-sectorial heat exchange between companies in industrial conglomerates and (nearby) district heating has been mentioned as an opportunity, but would of course add substantial complexity and poses additional challenges in supply security or could cause lock-in situations that prevent further efficiency measures on plant level. For this study, advanced heat integration is considered to be part of incremental improvement and implementation of BPT. In terms of heat pumps, this study includes steam recompression as technology in chapter 3.2.

2.4 Process-intensifying equipment

Process-intensifying equipment encompasses intensive mixing, heat-transfer and mass-transfer devices including structured reactors, advanced heat exchangers, mixers and enhanced (HiGee) or cold (e.g. membrane) separation equipment as well as integrated hybrid equipment such as reactive distillation, heat exchange reactors and membrane reactors.[13] The European Roadmap for Process Intensification quantifies enormous energy saving potentials for such equipment, but practical implementation is lagging behind, partly because of still

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[11] SPIRE Roadmap – Consultation Document, Sustainable Process Industry through Resource and Energy Efficiency (SPIRE), Brussels, Belgium, November 2012

[12] European chemistry for growth - Unlocking a competitive, low carbon and energy efficient future; Cefic, Ecofys, 2013

[13] See for instance: *Creative Energy, 2007 European Roadmap for Process Intensification, December 2007.*

existing technical issues, relatively small operating windows (of hybrid equipment) or large investment requirements.

2.5 Impact of efficiency measures

In light of the strong efficiency measures already implemented in the last decades and the relatively lower potential for the large petrochemical continuous processes which generally have reached high efficiency levels as opposed to many fine and specialty chemicals processes in batch, this study uses an improvement factor of 0.56% p.a. for further efficiency measures, which corresponds to the average factor that was also used in the IEA/ICCA/DECHEMA technology roadmap[6] as incremental improvement factor. This might be perceived as very conservative estimate, but two aspects have to be pointed out, that support this approach:

- the Cefic/Ecofys roadmap[12] confirms a stagnation in further efficiency improvements of the large petrochemical processes in recent years; improvements in the energy efficiency of ammonia plants in Europe over the last decade have been very low, between 2004 and 2011, even a slight decline of -0.17% per year was observed for 26 European ammonia plants. Likewise, only very small energy efficiency improvements have been made in the European steam crackers; an ambition of 0.56% improvement of the SEC is therefore not too pessimistic.
- Implementation of BPT or process intensification technologies potentially providing higher efficiency gains will usually be reserved to new production plants and hence subject to large investments. Investment decisions in favor of new plants using conventional fossil feedstocks will be in competition with similar investments in plants based on low-carbon technologies, that would preferably also be deployed in case of required new production capacities. In other words: new fossil-based plant capacities are likely to create a lock-in situation for breakthrough low-carbon technologies for several decades.

Table 2 shows the impact of efficiency measures in the different scenarios. Efficiency improvements as defined above are primarily taken into account for already existing plants, not for new plant capacities. As a consequence this kind of efficiency improvements takes place only for conventional processes, and the improvement potential decreases with the share of implementation of low-carbon technologies. Therefore, unlike the impacts for most of other low-carbon technology options, the effect is larger for the less ambitious scenarios.

Table 2: CO_2 reductions based on efficiency measures for the different scenarios

CO_2 reduction potentials due to efficiency measures	2015	2020	2025	2030	2035	2040	2045	2050
Interm [mill t]	0	2.1	4.2	6.2	8.1	9.5	10.8	11.9
Amb [mill t]	0	2.1	4.1	5.9	7.4	8.9	9.8	8.5
max [mill t]	0	2.0	3.9	5.2	5.2	4.5	3.5	2.5

3 Direct use of low-carbon electricity

This chapter deals with the use of electricity to either directly produce heat or upgrade sources of waste heat to useable temperature levels (Power-to-Heat) and chlorine production as electricity-based process. The indirect use of electricity to produce hydrogen and subsequent conversion with CO_2 (Power-to-X processes) is dealt with in chapter 4.

3.1 Electricity based steam production (TRL7)

A major part of the chemical industries' process energy demand is supplied as heat, i.e. steam at various temperature and pressure levels. The fuel used to generate steam accounts for 60% of the total fuel used in the chemical industry.[14] In 2014, the European chemical industry had a total consumption of derived heat of 319 PJ in 2014.[15]

Traditionally, chemical industry generates steam in natural gas fired boilers. The use of electricity in power-to-heat applications or hybrid boiler concepts switching between natural gas and electricity-based heating provides several advantages. Electricity based heating has a fast response time and can therefore flexibly be used to valorize intermittent surplus supply of renewable electricity. This way, chemical industry can offer an active contribution to the demand side management and enhanced flexibility of the power sector, and on the other hand chemical industry can benefit from periods with low electricity prices. This can be perceived as an element of industrial symbiosis between the chemical industry and the power sector.

A limitation of the use of electrical systems might occur for very high temperatures where conventional electric heating systems are limited or become very expensive[14], but this effect is considered less relevant for the processes considered in this study and is neglected in further analysis.

Generation of heat by combustion of natural gas (assuming 100% efficiency) accounts for emissions of 55.9 $kgCO_2/GJ$[16]. For the above mentioned 319 PJ this corresponds to 17.8 Mt CO_2-emissions. The emissions caused by electricity-based steam production strongly depend on the electricity mix, as shown in Figure 2.

Using grid-power, emission savings are achieved as soon as the decarbonization of the power sector is relatively advanced. For the IEA ETP 2°C scenario the break even is between 2030 and 2035. Earlier implementation is effective only if low-carbon power is employed, e.g. direct

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[14] Industrial Process Heating - Technology Assessment; https://energy.gov/sites/prod/files/2015/02/f19/QTR%20Ch8%20-%20Process%20Heating%20TA%20Feb-13-2015.pdf

[15] Source: eurostat

[16] German Environment Agency

use of electricity from a wind park. For the subsequent scenario calculations, CO_2 emissions for the electricity supply of 0.011 tCO_2eq/MWh have been used, corresponding to the IEA ETP 2°C power footprint in 2050.

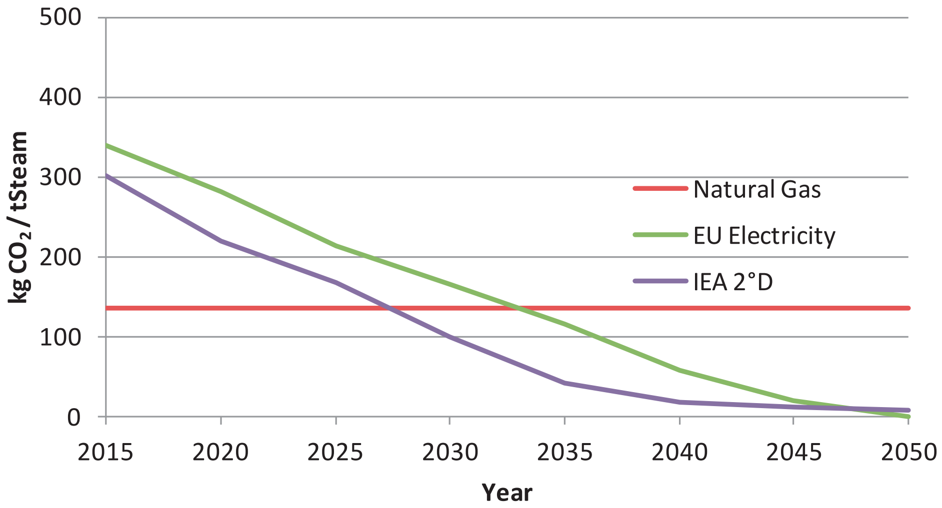

Figure 2: Emission profiles of electricity-based steam production (for anticipated EU electricity mix and IEA ETP2°C scenario) vs. steam from natural gas combustion

Furthermore, different effects have to be taken into account for the calculation of the future heat demand and potential GHG savings for electricity based steam production:

- the 1% increase in chemical production assumed in this study, which would call for a corresponding increase in heat demand; taking this and the around 60% share in energy demand of the considered large volume chemicals into account, the heat demand might rise to 393 PJ by 2050.
- the implementation of low-carbon technologies as projected in the different scenarios of this study will affect the availability of excess steam generated in some of the petrochemical processes: steam export is about 1.5 GJ per ton of product for naphtha steam cracking, 2 GJ/t for NG based methanol production and 4.3 GJ/t for NG based ammonia production[17]. For the electricity based low-carbon production processes, this excess steam originating from fuel combustion is not available; this amounts to 35 to 128 PJ additional heat requirement.

Based on these factors, heat demand and CO_2 reduction potentials have been calculated for the three scenarios. Table 3 summarizes the heat demand for the different scenarios and

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[17] Data from: IHS/IEA; IEA/ICCA/DECHEMA technology roadmap and Industrial Efficiency Technology Database (http://ietd.iipnetwork.org/content/ammonia)

calculates the potential CO_2 emission reductions based on the carbon footprint for power anticipated in the IEA 2°C scenario for 2050 as well as the electricity demand. The additional heat requirement due to increased production volumes and less available excess steam slightly reduces the achievable emission reductions. Higher ambitions in the low-carbon processes enhance this effect.

Table 3: Anticipated future annual steam demand as a result of the scenarios in this study

Heat demand	2015	2020	2025	2030	2035	2040	2045	2050
Accounting for increased production [PJ]	319	329	339	349	360	370	382	393
Total steam required, Interm [PJ]	319	329	339	351	364	381	402	425
Total steam required, Amb [PJ]	319	329	340	352	366	382	403	436
Total steam required, Max [PJ]	319	330	342	359	386	422	463	507
CO_2 reduction potentials	**2015**	**2020**	**2025**	**2030**	**2035**	**2040**	**2045**	**2050**
CO_2 emissions NG based [$MtCO_2$]*	17.8	18.4	18.9	19.5	20.1	20.7	21.3	22.0
Electrification; implementation rate	0%	2%	5%	15%	30%	50%	70%	100%
CO_2 reduction potential Interm [$MtCO_2$]	0	0.3	0.9	2.7	5.6	9.7	13.9	20.5
CO_2 reduction potential Amb [$MtCO_2$]	0	0.3	0.9	2.7	5.6	9.7	13.9	20.5
CO_2 reduction potential Max [$MtCO_2$]	0	0.3	0.9	2.7	5.6	9.6	13.8	20.2
Electricity demand, Interm [TWh]	0	2.0	5.2	16.2	33.3	57.2	82.5	121.4
Electricity demand, Amb [TWh]	0	2.0	5.2	16.2	33.7	58.8	86.8	131.2
Electricity demand, Max [TWh]	0	2.0	5.2	16.3	33.9	59.0	87.1	134.7

* for the baseline, no implementation of low-carbon technologies has been considered

3.2 Advanced heat management via steam recompression (TRL 6-7)

Most chemical processes demand low and medium level temperature steam. According to the Euroheat and Power industrial heat demand survey[18] (2006), the European chemical industry's low and medium temperature heat demand (100-400°C) is at least half of the total heat demand. A recent white paper initiated by the Netherland's VoltaChem Shared Innovation Program on the electrification of the chemical industry[19] estimates that about 35% of the final energy use for heat in the chemical industry is for heat at temperatures up to 200 °C, that can be obtained by heat pumps and upgrading of residual steam by mechanical vapor recompression. The white paper estimated 50% potential energy savings through application of these technologies, and 15-20% savings on energy for heat demand.

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[18] The European Heat Market, Euroheat & Power, 2006; https://www.euroheat.org/wp-content/uploads/2016/02/Ecoheatcool_WP1_Web.pdf

[19] Empowering the Chemical Industry, TNO and ECN 2016; https://www.tno.nl/media/7514/voltachem_electrification_whitepaper_2016.pdf

The heat content of steam is partially contained as sensible heat, i.e. proportional to the temperature difference and as latent heat defined by the phase transition between the liquid and vapor phase of water. Latent heat is in general the larger amount of heat stored in steam. In case of condensation, the latent heat content is released. However, if condensation takes place at a temperature level too low to be beneficial for the process of interest, its heat content is lost. Steam recompression avoids unbeneficial condensation by compressing the low temperature low pressure steam before condensation occurs, thereby avoiding the energetic penalty to re-evaporate water. Avoiding these specific condensation losses can significantly enhance the efficiency of an integrated steam system and thereby increasing the overall efficiency of the production site and the integrated processes. However, steam recompression is investment intensive and currently only considered for large integrated site with steam consumption of at least 25 t/h. Steam recompression is currently evaluated at demonstration level in integrated chemical sites. Dow Benelux has completed an economic feasibility study of the use of mechanical damp recompression, where steam is upgraded by using electricity[19], and is now piloting the technology.

In effect, steam recompression acts as a highly efficient heat pump with a coefficient of performance between 5 and 10, depending inversely on the temperature difference. If 10% of the total consumption of derived heat (319 PJ today) is accessible to be generated by steam recompression, this would amount to 32 PJ. Assuming a coefficient of performance of 5 to 10, an electrical input for the actual compression of 6.4 PJ (1777 GWh) or 3.2 (889 GWh) of electric energy would be required.
At the emission level of current electricity generation (0.387 tCO_2/MWh) this corresponds to 690 kt and 344 kt CO_2-emissions respectively, compared to 1.780 kt CO_2-emissions caused by combustion of natural gas to generate the same amount of heat. Even with today's EU electricity mix, the potential reduction of CO_2-emissions for heat generation at full implementation would therefore amount to 1.090 kt or 1.436 kt respectively, roughly 1% of the CO_2-emissions currently allocated to the chemical sector (132 Mt CO_2). This number is expected to increase to roughly 2.2 Mt CO_2 with the decarbonisation of the power sector. Table 4 summarizes the potential impact for the three scenarios assuming power decarbonisation as foreseen in the IEA 2°C scenario. Differences between the scenarios of this study are negligible.

Table 4: Potential impact of steam recompression on CO_2 emission reduction

Steam re-compression	2015	2020	2025	2030	2035	2040	2045	2050
Implementation rate	0%	2%	5%	15%	30%	50%	70%	100%
CO_2 reduction potential Interm [$MtCO_2$]	0	0.03	0.08	0.27	0.59	1.02	1.48	2.19
CO_2 reduction potential Amb [$MtCO_2$]	0	0.03	0.08	0.27	0.59	1.02	1.48	2.18
CO_2 reduction potential Max [$MtCO_2$]	0	0.03	0.08	0.27	0.59	1.02	1.48	2.18

Full implementation of the electricity based steam generation and upgrade of waste heat is foreseen for all scenarios, as these technologies represent relatively easy to implement entry points for the electrification of the chemical industry. For steam re-compression, at current prices for natural gas (8.18 €/GJ [IEA]) savings in fuel from 190 Mio. €/a to 225 Mio. € (electricity price 40 €/MWh) could be realized already today, making this technologies economically attractive.

3.3 Chlorine production (TRL 9)

Chlorine production can be considered as a special case in the sense as this process is already based on electricity. The process carbon footprint is largely determined by the carbon footprint of the employed electricity mix. In this sense, low-carbon chlorine production will rely on the decarbonisation of the power sector.

3.3.1 Process scheme of chlorine production

Industrial chlorine is produced by the electrolysis of aqueous sodium chloride, called the chloralkali process. Besides chlorine, hydrogen gas and sodium hydroxide are also produced. Chlorine production is dominated by three different process technologies: membrane cell, mercury cell and diaphragm cell process. An abbreviated general process scheme is depicted in Figure 3.

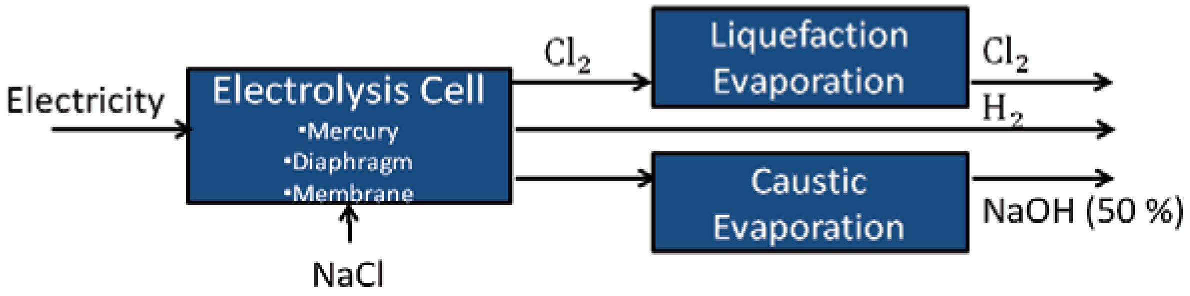

Figure 3: Generalized process scheme for the production of chlorine

In the membrane cell process, the anode and the cathode are separated by an ion-exchange membrane, through which only sodium ions and a little water pass. In the mercury cell process, sodium forms an amalgam (a mixture of two metals) with mercury at the cathode. The amalgam reacts with water in a separate reactor (decomposer) where hydrogen gas and caustic soda solution at 50% strength are produced. The mercury cell process also emits small amount of mercury. In the diaphragm cell process the anode area is separated from the cathode area by a permeable diaphragm. The brine is introduced into the anode compartment and flows through the diaphragm into the cathode compartment. All three technologies produce hydrogen and caustic soda, the latter in different concentrations (diaphragm: 11%, membrane: 32%). In case of diaphragm or membrane technology, steam is used to increase the concentration of the caustic to market specifications (50%). European mercury cell plants are expected to phase out by 2017. The existing plants are continuously either decommissioned or reconditioned to the membrane cell process.

Recently installed new membrane cell capacities (2009) can e.g. be found in Spain (30 kt per year) and Germany (430 kt per year). Since 1984, no new plants based on the mercury cell technique have been built and only a few diaphragm cell plants. For existing chlorine plants, the following measures have to be considered:

- Conversion of mercury cell plants to membrane cell technology: by this, electricity consumption is reduced by about 23%. However, additional steam is required to concentrate the caustic soda to 50%, as the produced caustic soda in membrane cell technology has a lower concentration (32%) than in mercury cell processes. The main driver for the conversion to the membrane technology is a voluntary agreement and 100% transition is expected to be complete in Europe by the end of 2017.
- changing monopolar to bipolar membrane technology: this applies only to membrane cell processes. Bipolar cells save energy by minimising the inter-cell voltage losses. The current share of monopolar technology in membrane cells is approximately 10%, which means the maximum applicability of this measure is about 5% of total chlorine capacity.
- retrofitting of membrane cell plants to oxygen-depolarised cathodes (ODC) technology: ODC can be used in membrane cell processes and reduce oxygen to produce hydroxide instead of converting water to hydrogen and hydroxide. This lowers the cell voltage by about 1 volt and translates to an energy saving of about 30%. The actual saving is lower, as oxygen with high purity needs to be produced, and hydrogen is no longer coproduced, which is a key component for the low-carbon technologies described in chapter 4; A membrane cell plant using the ODC technique operated by Bayer and UHDENORA / Uhde with a chlorine capacity of 20 ktons per year was put into operation in summer 2011.

Chlorine production co-produces hydrogen in significant amounts. Hydrogen can either be used as chemical feed in downstream processes or burned to cover additional heat requirements in the plant, e.g. raising the concentration of the caustic soda product to its market specification (50 %).

3.3.2 Energy demand per unit of production

The specific energy demand depends on the process technology. It covers the following aspects:

- Electrical energy demand for the electrolytic reaction

- Additional electric demand for auxiliary processes
- Heat requirements to promote caustic soda to market specifications

Table 5 shows the energy consumption for the different chlorine production technologies. The energy demand for the electrolysis cell is the energy demand per electrochemical unit, i.e. the coproduction of chlorine, caustic soda and hydrogen. Burning hydrogen can be used to cover additional heat requirements of the process. Excess hydrogen can also be reconverted by means of a fuel cell to electrical energy.

Table 5: Energy consumption (median) of chlorine production within the EU and EFTA[20]

Process	Electrolysis Cell	Other electrical equipment	Caustic soda concentration
Mercury	3400 kWh/tCl_2	200 kWh /tCl_2	0
Diaphragm	2800 kWh/tCl_2	200 kWh /tCl_2	2.8 GJ/tCl_2
Membrane	2600 kWh/tCl_2	200 kWh /tCl_2	0.7 GJ/tCl_2
Membrane / ODC	1800 kWh/tCl_2	200 kWh /tCl_2	0.7 GJ/tCl_2

Future development of chlorine production technology is expected to reach 2400 kWh/tCl_2 for the power consumption by 2050, while the energy requirement for caustic soda generation is expected to remain constant [21].

3.3.3 CO_2 emission reduction per unit of chlorine production

Chlorine production does not release any process-specific CO_2 emissions. The overall amount of CO_2-emissions depends on the specific CO_2-emissions per unit of electrical energy required. The EU CO_2-emission intensity for power generation (2013) was 558 g/kWh_{el} [22]. Under the assumption, that all energy requirements of the chlorine plant are met by electricity, the corresponding specific CO_2 emissions related to the production of 1 ton of chlorine are given in Table 6.

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[20] Thomas Brinkmann, Germán Giner Santonja, Frauke Schorcht, Serge Roudier, Luis Delgado Sancho; JRC Science and Policy Reports “Best Available Techniques (BAT) Reference Document for the Production of Chlor-alkali”, 2014

[21] CEFIC, Ecofys „European chemistry for growth“; 2013

[22] http://www.eea.europa.eu/data-and-maps/indicators/overview-of-the-electricity-production-1/assessment

Table 6: CO_2-emissions related to the production of chlorine based on 558 g/kWh

Process	Total electrical energy requirement	Corresponding specific CO_2-emissions
Mercury	3600 kWh/tCl_2	2.0 tCO_2/tCl_2
Diaphragm	3800 kWh/tCl_2	2.1 tCO_2/tCl_2
Membrane	3050 kWh/tCl_2	1.7 tCO_2/tCl_2
Membrane / ODC	2250 kWh/tCl_2	1.3 tCO_2/tCl_2

Since the specific CO_2-emissions for the production of chlorine are a direct function of the CO_2 intensity of the power generation, they are expected to decrease in conjunction with increasing introduction of low-carbon power generation. Additional emission reduction beyond reducing the electrical energy requirement of the processes and general decline of CO_2-emission intensity of electrical power can only be achieved by a dedicated supply of low-carbon electricity to the chlorine plants. Table 7 summarizes the expected emissions from the European chlorine production. The carbon footprint of power generation used in the calculations has been assumed to follow the IEA ETP 2°C scenario.

Table 7: Chlorine production and expected emissions based on expected decarbonisation of the power sector (IEA ETP2°C scenario)

Chlorine impact	2015	2020	2025	2030	2035	2040	2045	2050
Chlorine production [mill. t][23]	9.58	10.07	10.58	11.12	11.69	12.28	12.91	13.57
Emissions [mill. t]	11,4	10.0	8.1	5.02	2.19	1.04	0.72	0.55

In terms of power consumption and CO_2 emissions, ODC is distinctly below the other technologies. On the other hand, ODC does not deliver hydrogen. Stoichiometrically, the membrane chlorine process delivers 28.4 kg hydrogen per ton of chlorine. Considering the hydrogen-based technologies described in chapter 4 and the expected large demand for hydrogen in the future, hydrogen from chlorine production would probably have a much higher valorization than today. Hence, a further extention of current ODC capacities has not been assumed for this study.

3.3.4 Chlorine process economics

Chlorine production is a capital intensive process at the beginning of various value chains for it products (chlorine, hydrogen, caustic soda). Electricity is considered as raw material rather than utility cost and amounts for around 50% of the specific production costs to produce chlorine and caustic soda. Table 8 provides estimated investment costs taken from different studies and reports. As already stated in the introduction, a low-carbon chlorine production relies on the decarbonisation of the power sector and no specific actions or additional investments by the chemical industry are necessary.

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[23] 2015 production taken from Eurochlor; development based on 1% growth p.a.

Table 8: Investment costs for chlorine plants.

Process	Investment costs yearly capacity
Mercury	500 €/tCl_2
Diaphragm	540 €/tCl_2 [24]
Membrane	500 €/tCl_2 [25] (1100-1500 €/tCl_2) [26]
Membrane (conversion from mercury)	360-560 €/tCl_2 [27]
Membrane / ODC	660 €/tCl_2
Membrane / ODC (retrofit)	100 €/t Cl_2

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[24] http://insights.globalspec.com/article/855/changing-regulations-and-energy-costs-impact-the-global-chlor-alkali-industry assumes 8% cost advantage of membrane vs. diaphragm

[25] As of http://www.chemicals-technology.com/projects/dowmitsuichloralkali/

[26] Frank Holtrup, WEC, „Potenzial für Demand Side Management der energieintensiven Industrie in Deutschland“ reports these values.

[27] European Commission, “An economic and environmental analysis of the chlor-alkali production process”, 1997

4 Hydrogen/CO_2-based production routes

The chemical industry is based on transformation processes, where carbon and hydrogen are essential elements. Reactions with mixtures of hydrogen, carbon monoxide and carbon dioxide are well known in the chemical industry as synthesis gas-based routes, and they can be used to build-up all major platform chemicals for the chemical industry's value chain. In contrast to the usual gasification processes to convert fossil carbon feedstocks into synthesis gas, subject to the corresponding high CO_2 emissions, alternative pathways can be designed using hydrogen from low-carbon electricity as a reactant. From the nine target products considered in this study, ammonia can be directly synthesized using hydrogen and nitrogen. For the other (organic) petrochemical products (i.e. methanol, the olefins ethylene and propylene and BTX), but also synthetic fuels a carbon source is required, and carbon dioxide can serve as such a source, currently available as end-of-pipe waste from more or less concentrated point sources such as flue gas of fossil-fired power plants, industrial processes such as lime/cement production, steel manufacturing but also within the chemical industry. In effect, these routes offer an opportunity for the chemical industry to reduce its dependence on fossil fuels, to reduce industrial CO_2-emissions as well as to recycle and valorize emitted CO_2. The long term availability of CO_2 is considered in chapter 4.10.

Hydrogen acts as a key high-energy containing reaction partner in the conversions of CO_2 to the aforementioned target products, this energy being necessary to activate and convert the both kinetically inactive and thermodynamically stable carbon dioxide molecule. Realizing a low-carbon chemical industry therefore requires a shift in the production of hydrogen from the classic steam reforming of methane to new, CO_2 lean, technologies. Different routes to produce low-carbon hydrogen are available, and this chapter will start looking at these technologies.

Other conversions with CO_2, not including hydrogen, are not covered here, but are briefly described in chapter 5. These include transformations with alternative high-energy containing reactants such as epoxides and unsaturated compounds or the conversion of CO_2 into target molecules with even lower energy content than CO_2, e.g. organic carbonates and polymers.

4.1 H_2 production via low carbon emission routes

Different routes to produce low-carbon hydrogen are available and water is the usual source for hydrogen. The reaction pathways depend on the concrete setup of the technique but the net reaction can be summarized as

Water splitting: $2\ H_2O \rightarrow 2\ H_2 + O_2 \qquad \Delta H^0 = 571.8$ kJ/mol.

The high ΔH^0 value indicates the intense energy requirement of the water splitting, which makes H_2 production usually the most energy demanding step in the production of chemicals from H_2 and CO_2.

4.1.1 Electrolytic production of hydrogen

Water can be split into its elements, hydrogen and oxygen by applying an electric current. The principle has long been used for industrial hydrogen production. The CO_2-footprint of this hydrogen production rests essentially with the CO_2-emissions of the respective power generation process. Therefore, none of these routes will have a positive impact on the overall CO_2-emissions unless the electricity used is based on low-carbon power generation and not being compensated for by fossil fuel based power generation within the power sector. With progressing decarbonisation of the power sectors, electrolytic technologies offer a pathway to introduce low-carbon production pathways into the chemical sector.

Electrolytic processes are identical to fuel cell processes, with the direction of the electrochemical reaction reversed. All of the following processes can therefore in principle be also operated reversely in a fuel cell mode. However, technical requirements differ significantly between the electrolytic technologies. There are three main technical routes for electrolytic hydrogen generation.

4.1.1.1 Alkaline Electrolysis (TRL: 7-9)

This is the state-of-the art industrial process for electrolytic hydrogen production. Rather than pure water, a 20-40% solution of KOH is used and the electrodes are coated with Ni as catalyst. Both half-cells are separated via a diaphragm to prevent mixing of the gases. Alkaline electrolysis can be applied at normal pressure or under pressure of up to 30 bars. Efficient plants require 4.3 kWh per Nm^3 of H_2 which amount to a conversion efficiency of around 70%. About 4% of the global hydrogen production is based on this process. Alkaline electrolysis is available at commercial scale at system costs of 1000-1200 €/kW[28] and system size up to 5.3 MW per stack.

In terms of further technical advancements by 2050, a few percentage points in the area of efficiency can be expected. More importantly, major reductions in the investment costs for alkaline electrolysis plants will remain in the focus of development efforts. Materials development for electrodes to reduce overpotentials and to allow higher current densities at a given cell voltage are expected to contribute to an overall increase in efficiency. Additional experience needs to be acquired for safe operation in uncommon process windows, such as in combining fluctuating and intermitting power sources with large scale alkaline electrolysis is

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[28] Study on development of water electrolysis in the EU, E4tech and Element Energy Ltd or the Fuel Cells and Hydrogen Joint Undertaking, February 2014, p. 12-13.

required, especially with respect to safety, operational windows and long-term stability of materials and components. Even if alkaline electrolysis can be regarded as a ‘mature’ technology, production volumes are still low, and it is expected that cost reductions can be leveraged from an improved supply chain, and through increased production volumes.
Alkaline electrolyser systems cost are expected to reduce to about 600 €/kW by 2030. More optimistic estimates see alkaline electrolyser costs approaching 370 €/kW[28]. For this study, the latter number is considered as more realistic for 2050.

4.1.1.2 PEM-Electrolysis (TRL: 7-8)

PEM (Proton-Exchange-Membrane) electrolysis has been developed in the last 20 years. In contrast to the alkaline version, it runs on pure water and no treatment / recycling of the KOH solution is necessary. PEM stacks are very compact and can be designed for high pressures up to 100 bars. PEM electrolysis also demonstrates a very good dynamic behavior, which allows them to follow, for example, the power-profile of a wind turbine without significant delay. Again, the main drawbacks of this technology are the investment costs which are dominated by the high costs for catalyst materials like Pt and Ir. First units are now successfully operating for some years, but no full life-cycle has been experienced under operational conditions. This technology is at the core of Audi’s E-Gas project, where wind turbines provide electricity for a PEM electrolyser. Hydrogen then reacts with CO_2 separated from biogas to produce methane which is fed into the natural gas grid[29].

For PEM electrolysis, investment costs are expected to drop significantly as production experience increase and alternative cheaper catalysts are developed. Current PEM electrolyser installations reach up to 6 MW power. Further technological development is expected to boost the performance of this technology significantly and therefore enhance the installed capacities by at least one order of magnitude.
The system cost of PEM electrolysers is currently about twice that of alkaline systems. Costs at around 1,000 €/kW are expected by 2020, although several manufacturers anticipate costs near 700 €/kW[28]. Further reductions by 2030 and beyond might result in costs of 500 €/kW.

4.1.1.3 High-temperature solid-oxide electrolysis (TRL: 6-7)

The amount of electricity required to split water into its elements can be reduced by operating the electrolysis at a higher temperature, around 700-1000°C, which can reduce the electricity requirements down to 2.6 kWh per Nm^3. This temperature range requires different materials and the cell membrane is a ceramic material capable of conducting oxygen ions. Industrial

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[29] The first industrial PtG plant – Audi e-gas as driver for the energy turnaround, Reinhard Otten, CEDEC Gas Day, Verona, May 2014

sites with significant waste heat sources at high temperature can harvest the advantages of this technology. *sunfire*, a Germany-based company has successfully coupled hydrogen generation via high-temperature solid-oxide electrolysis (SOE) with a Fischer-Tropsch reactor as heat source and to transform the generated hydrogen with CO_2 to car fuels.[30]

High-temperature solid oxide electrolysis is expected to find applications where high-temperature heat sources can be tapped. Operation and maintenance will require specialists for the foreseeable future and its deployment therefore most likely closely linked to existing industrial sites. Additional improvements in the area of materials and system integration are expected to lift TRL up to 9 by 2030. For SOE, literature suggests that systems might become available between 2015 and 2020 at a cost of roughly 2,000 €/kW, while the cost would approach 1,000 €/kW between 2020 and 2030 and might reach 300 €/kW in the longer term.[28]

4.1.1.4 Water electrolysis technical performance and system cost

Table 9 shows a comparison of different technical and economic factors for the different electrolyser technologies and expectations towards the future, taken from different studies. As benchmark, steam methane reforming (SMR) as state of the art technology for hydrogen production is also included.

Table 9: Electrolyser technologies, performance and CAPEX costs today and in future

	Parameter		Alkaline	PEM	SOE
Today	Investment costs €/kW		1000-1200[28] 800-1500[31] 650-1200[32]	1860-2320[28,32] 2000-6000[31]	>2000[28]
	OPEX costs		2-5% of CAPEX[28]	2-5% of CAPEX[28]	2-5% of CAPEX[28]
	System sizes	Nm^3 H_2/h	0.25 – 760[28]	0.01 – 240[28]	40[33]
		kW	1.8 – 5,300[28]	0.2 - 1,150[28]	100[33]
	Efficiency kWhel/kgH_2		50 - 73[28]	47 - 73[28]	37[33]
2030 and beyond	Investment costs €/KW		600[28] 800[34] 370-800[32]	500[28] 700[34] 250-1270[32]	300-1000[28] 625[32]

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[30] http://www.sunfire.de/en/applications/fuel

[31] Power to Gas system solution. Opportunities, challenges and parameters on the way to marketability. Dena 2015; http://www.powertogas.info/fileadmin/content/Downloads/Brosch%C3%BCren/dena_PowertoGas_2015_engl.pdf

[32] Commercialisation of energy storage in Europe, final report, 2015, http://www.fch.europa.eu/sites/default/files/CommercializationofEnergyStorageFinal_3.pdf

[33] sunfire; http://www.sunfire.de/en/products-technology/reversible-generator

[34] IEA Technology Roadmap Hydrogen and Fuel Cells, 2015

	Hydrogen production costs [€/kgH_2]	4.5 (500 Nm^3/h, 98 % utilisation,, 0,075 €/kWh)[35]	3.17 (250 Nm^3/h 98% utilisation, 0,05 €/kWh)[35]	
		Further reduction down to to 2€/kgH_2 indicated[35]		
	System sizes	500 MW installations	MW stacks	MW stacks (long term)
	Efficiency kWhel/kgH_2	48 - 63[28]	44 - 53[28]	37
SMR	Investment costs [€/kW]	520-780[36]		
	System size [MW]	150-300[36]		
	Efficiency	70-85% (LHV)[35]		
	Hydrogen production costs	see chapter 4.1.1.5, Figure 5		

Investments costs are expected to decrease with further innovation and research focusing on cost reductions as well as (limited) economy-of-scale effects when significant deployment takes place. Nevertheless economy of scale effects are limited in electrolysis compared to other technologies, as electrolysis is a surface process and the system size almost linearly increases with the cell area. This means that scale-up is to a large degree realized by numbering-up of stacks. Smolinka et al.[35] indicate that larger systems can achieve some cost advantages with regard to balance of plant (e.g., inverter, gas drying, system control), when going from kW systems up to 500 kW, the effect will however flatten after this point. Electrolyser efficiency (as energy input in kWh per kg of hydrogen output) will further increase but only moderately. The theoretical minimum electrical energy input is 39.4 kWh/kg H_2 (HHV of hydrogen). In case of SOE, the electrical input can even be lower, if water is supplied as steam using suitable process heat sources.

4.1.1.5 Hydrogen production costs

Production costs of hydrogen strongly depend on two main factors: i) electricity costs and ii) utilisation rate of the electrolyser (operating time, particularly relevant in case renewable electricity is used and supply is fluctuating). Smolinka et al.[35] have investigated the sensitivity of hydrogen production costs as a function of the utilisation rate and other factors and showed a cost range of 3-9 €/kg H_2 for different scenarios. The relative CAPEX costs can be quite high at low utilisation rates, 65% and more, and a factor of 5 in hydrogen production costs was observed depending on the utilisation rate, showing a strong need to ensure a continuous operation.

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[35] Smolinka et.al., NOW-Study: Stand und Entwicklungspotenzial der Wasserelektrolyse zur Herstellung von Wasserstoff aus regenerativen Energien, Fraunhofer ISE, 2011

[36] Data from “Technology Roadmap Hydrogen and Fuel Cells”, IEA 2015

The cost of hydrogen as a function of the operating hours of the electrolysis equipment is depicted in Figure 4. The calculation provided for alkaline and PEM electrolysis was performed using data from the IEA Technology Roadmap Hydrogen and Fuel Cells.[37]. Details are provided in Annex 1. Cost strongly increase at very low operating hours; efficiency, size and investment cost are other factors determining the cost range.

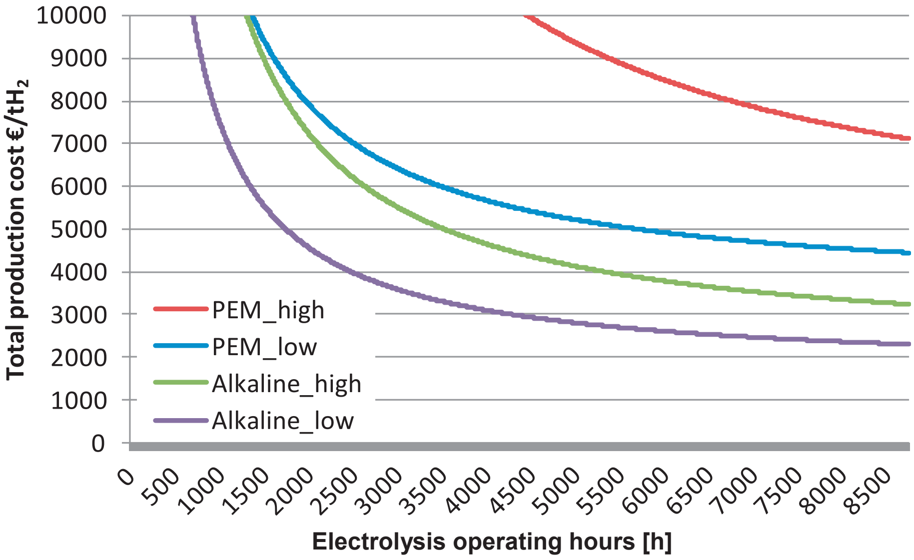

Figure 4: Cost sensitivity of hydrogen from PEM and alkaline electrolysis as a function of operating hours; based on Ref. 37 for an assumed electricity price of 40 €/MWh

Figure 5 shows the cost of hydrogen production for methane steam reforming in comparison with PEM and alkaline electrolysis at full operating hours based on the same cost of energy for the different options, showing the economic gap of nearly factor 2 for alkaline or even higher for PEM electrolysis. Cost reduction is therefore an absolute priority for future innovation.

The opportunistic use of cheap electricity, e.g. during periods of surplus renewable electricity supply, would lead to a significantly low utilisation of the assets with detrimental effect on economics. The discussed high investment technologies are disadvantageous for low utilisation rates.

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[37] https://www.iea.org/publications/freepublications/publication/TechnologyRoadmapHydrogenandFuelCells.pdf

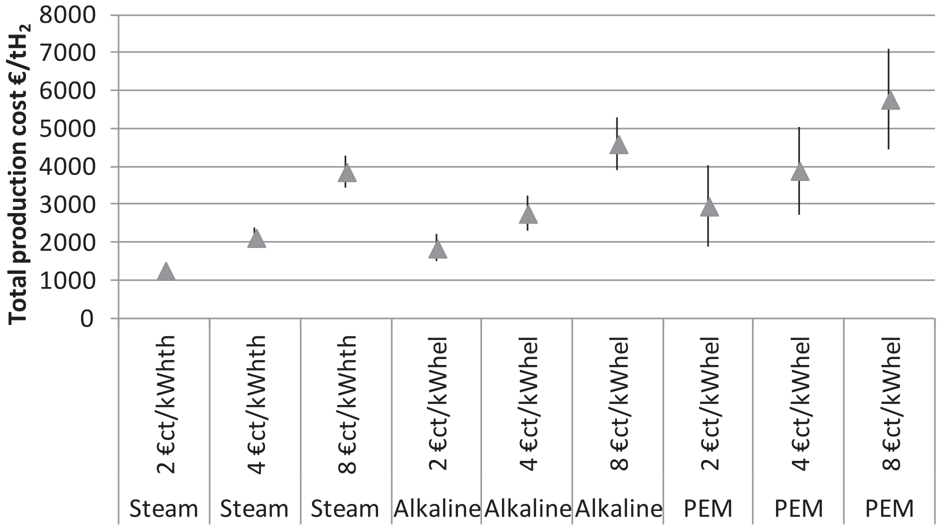

Figure 5: Cost comparison hydrogen production cost for methane steam reforming (steam) and electrolyser technologies (Alkaline, PEM)

4.1.1.5 Electrolysers and future scale for chemical production

A simple calculation shows how the scale of chemical production needs to be matched to a reasonable scale of electrolysers.

Typical size for methanol production plants (MegaMethanol, GigaMethanol plants) are in the range of 3000 -10000 tons per day At a stoichiometric hydrogen demand of 189kg H_2/t methanol, an electrolyser would need to deliver 560-1900 t (or 6.6 -22 mill. Nm^3) hydrogen per day. The electricity demand of such an electrolyser unit would be 28 - 95 GWh/d and an installed power of 1.3 – 4.3 GW would be necessary at continuous (8000 h/a) operation, corresponding to 1-4 large power plant units. This corresponding power would need to be supplied by low-carbon sources such as renewable, in order to allow a low-carbon chemical production. The electrolyser plant footprint would be at least 1000x700 m^2 [38].

Chemical production plants based on hydrogen generated by water electrolysis are therefore likely to be realized in smaller, decentralized installations rather than world-scale type production plants. The already mentioned fact, that electrolysers can only leverage moderate benefits from scale effects is advantageous in this respect, however, the relative capital investments of the chemical production plants will increase, as economy of scale is reduced. The optimum size may differ from local specific infrastructures, availability of low-carbon electricity, CO_2 source, industrial symbiosis opportunities with other industry sites nearby etc.

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[38] H.-J. Fell, NEL Hydrogen, NOW workshop Berlin, 2011; a 578 MW alkaline electrolysis concept of Norsk Hydro, containing 248 modules has a plant footprint of 550x350 m^2

4.1.1.6 Carbon footprint of hydrogen from low-carbon electricity

Hydrogen produced from low-carbon electricity is not carbon neutral. Even for renewable electricity a carbon footprint has to be allocated. For instance, the carbon footprint of electricity cradle to gate from a wind power plant encompasses the wind turbine production (e.g. accounting for steel and concrete used in its construction), operation of the wind power plant and transport of the electricity to the fence of the industrial site. Ecoinvent data suggests a carbon footprint of 11.2 g CO_2eq/kWh for a wind power plant including infrastructure[39]. For delivering 1 ton of hydrogen at 4.3 kWh/Nm^3, 50.4 MWh electricity are required, corresponding to a footprint of **0.56 tCO_2eq**. This is the carbon footprint per ton of hydrogen for low-carbon hydrogen production used in the subsequent sections of this study. A partial allocation of this carbon footprint to oxygen as the by-product of water electrolysis is not considered, as a use and hence specific value of this oxygen has not been identified within the framework of this study.

It should be mentioned that other authors performing a complete LCA on hydrogen from renewable electricity also included electrolyser construction and operation with 0.043 kg CO_2e/kg H_2 and hydrogen compressors and storage tanks with 0.17 kg CO_2e/kg H_2 in their calculations[40] These relatively low impacts are disregarded in this report for simplicity reasons, as similar considerations would also be necessary for the conventional fossil processes, adding a high level of complexity to the analysis. Table 10 summarizes these numbers.

Table 10: Carbon footprint of hydrogen production

Electrolysis		Carbon footprint (CF) [tCO_2eqtH_2]	
Efficiency [kWh/Nm^3 H_2]	4.3	CF of required power at 11.2 g CO_2eq/kWh, used as benchmark in this study	**0.56**
Required power [MWh/ tH_2]	50.4	construction and operation of assets, not included in the study	0.213

4.1.2 Alternative low carbon hydrogen production processes

Apart from electrolysis, several other processes can be used to generate hydrogen. These processes are described subsequently.

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[39] Ecoinvent unit processes wind power plant/RER

[40] P. L. Spath, M. K. Mann, 2004: Life Cycle Assessment of Renewable Hydrogen Production via Wind/Electrolysis. Milestone Completion Report-NREL/MP-560-35404.

4.1.2.1 Methane pyrolysis (TRL 4-5)

The thermal decomposition of methane is a promising emerging route towards the production of hydrogen with a low carbon footprint. Methane or other lower hydrocarbons are decomposed in a high temperature pyrolysis process generating hydrogen and solid carbon. It can be summarized as:

$$CH_4 \rightarrow 2\ H_2 + C\ \Delta H_R^0 = 37{,}4\ \text{kJ/mol}\ H_2.$$

The enthalpy of reaction is significantly lower than for water splitting leading to much lower energy demand for hydrogen production. Like for water electrolysis, no direct CO_2-emissions are generated in the reaction and the required energy can be supplied by electricity. The methane feedstock could stem from fossil sources, but also biogas, landfill gas or synthetic methane. The type of carbon product depends on the applied technology and can be discussed for utilisation e.g. in tire manufacturing, reducing agent in metallurgical processes or can be discussed for storage. The carbon use generates a commercial benefit for the hydrogen production and also replaces other fossil raw material sources in industrial areas other than the chemical industry. Based on today's electricity generation mix, the carbon footprint for hydrogen and carbon production can be reduced by ~50% if carbon use and heat integration within the process is successful. If the – only indirect emissions – are allocated to hydrogen and carbon, an even higher reduction for hydrogen is achieved. Different technical approaches are followed and R&D and pre-commercial projects for example thermal decomposition by a consortium of BASF, Linde and ThyssenKrupp[41] and plasma pyrolysis by the US-based company Monolith[42] are ongoing. Other approaches include thermocatalytic decomposition (Muradov) or liquid metal processes (KIT, IASS). Since methane pyrolysis is only partly in pre-commercial state, it is not taken into account for the scenario calculations in the study.

4.1.2.2 Thermochemical processes (TRL: 4)

Splitting of water can also be achieved by high-temperature heat. However, the temperature requirement for direct water splitting process of more than 2000°C needs to be reduced by catalytic thermochemical cycles. Many materials can serve as catalyst as long as they match the redox-chemistry and stability requirements at the process temperatures. Thermochemical processes also exist for the splitting of CO_2. In combination, these processes allow the generation of synthesis gas. As for electrolytic hydrogen generation, the question of sustainability or carbon-neutrality rests with the heat generation. Solar heat or waste heat would be preferable.

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[41] A. Bode, D. W. Agar, K. Büker, V. Göke, M. Hensmann, U. Janhsen, D. Klingler, J. Schlichting, S. A. Schunk, in Proc. of the World Hydrogen Energy Conference, Gwangju, June 2014.

[42] http://monolithmaterials.com/

Thermochemical processes have been developed for solar heat supplies. The concept is well proven but should also be considered for high-temperature industrial waste heat, where new reactor concepts need to be developed. New catalytic thermochemical cycles are expected to reduce temperature requirements. The efficiency and durability of reactant materials for thermochemical cycling need to be improved. Efficient and robust reactor designs compatible with high temperatures and heat cycling need to be developed. For solar thermochemical systems, the cost of the concentrating mirror systems needs to be reduced. Demonstration scale process will probably emerge by 2050.

4.1.2.3 Photocatalytic processes (TRL: 2-3)

Photocatalytic reactions use solar light energy to split water at the surface of a catalyst. A lot of fundamental research activities have been dedicated to various concepts of photocatalytic water splitting. Current materials do not display sufficiently high yields for technical processes and still tend to work best at the ultraviolet part of the solar spectrum. One of the most well-known photo-catalysts used is TiO_2, but also has drawbacks, such as the need to add sacrificial agents into the solution. A number of reviews are available on the topic.[43]

This technology is not at pilot stage yet and has therefore not been considered in the scenarios of this study.

4.1.2.4 Hydrogen from other industrial processes

Several processes in the chemical and petrochemical industry produce hydrogen in various degrees of purity as side streams. Depending on the site structure, this hydrogen might enter other processes, be captured and sold or just being flared. Chlorine production has already been mentioned in chapter 3.3. Refineries generate and use hydrogen on-site to desulphurise their feedstocks and to upgrade their fuels.

Other industrial sectors, like steel, produce significant amounts of hydrogen-heavy off-gases that generally get burned to provide process heat. Some of these processes might add potential to a close cooperation between different sectors for a more efficient use of resources.

Hydrogen is mostly used as “captive” hydrogen that is on the same industrial site. Estimates assume 90 % of global hydrogen production being used on site and only a relatively small amount being sold and transported over the fence. Further details on this aspect are discussed in chapter 7 on industrial symbiosis.

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[43] H. Ahmada, S.K. Kamarudina, L.J. Minggua, M. Kassim, Hydrogen from photo-catalytic water splitting process: A review; Renewable and Sustainable Energy Reviews 2015, 43, 599–610.

4.2 Ammonia production from hydrogen

Ammonia ranks second, to sulfuric acid, as the chemical with the largest tonnage of the chemical industry globally. European ammonia production is currently at 17 million tons p.a.[44]. Ammonia production is closely related to food production and hence world population, demand will increase further accordingly. Over 80% of the ammonia produced worldwide is currently utilised in fertilizers, mainly urea and ammonium salts, for food production. 5% is used for nitric acid production. Another important product is acrylonitrile. Furthermore, ammonia serves as a building block in many pharmaceuticals and in cleaning products.

4.2.1 Conventional ammonia production (TRL 9)

Up to date, ammonia is nearly exclusively produced in large scale plants (up to 3.300 tons per day) from hydrogen and nitrogen on a Fe-based catalyst at 150 - 350 bar and 450 - 550 °C in the Haber-Bosch process.

Ammonia Synthesis: $N_2 + 3\,H_2 \rightarrow 2\,NH_3 \qquad \Delta H^0 = -46.22$ kJ/mol

Natural gas is the most relevant feedstock in Europe. Stoichiometrically, CO_2 is formed as co-product at 0.97 t CO_2 per t of NH_3 produced. In reality, average direct CO_2 emissions of European ammonia plants amount to 1.33 t/tNH_3.[45] As long as the hydrogen is supplied by methane steam reforming (or other fossil sources, this feedstock related CO_2 emissions are unavoidable. However, a large proportion of the CO_2 is subsequently used for the production of urea.

Simplified, the process includes the following steps: After a desulphuration step, the feed gas is mixed with process steam in the primary reformer, in which about 60% of the natural gas feedstock is converted to syngas in a highly endothermic reaction. Typical fuel use in the primary reformer (including steam generation) ranges between 7.2 and 9.0 GJ/ton of ammonia. The secondary reformer completes the feed reforming by internal combustion of part of the reaction gas with supplied air, which is also the source of nitrogen. The process gas exiting the secondary reformer contains 12-15% of CO which is converted with water in the shift converter into carbon dioxide and additional hydrogen. Following the removal of acid gas, the actual ammonia synthesis is performed by hydrogen reacting with nitrogen on an iron catalyst at a pressure of 150-350 bar and temperature of 350-550°C. Including the required oxygen, the overall chemical reaction would then be:

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[44] IFA, http://www.fertilizer.org/en/doc_library/Statistics/PIT/ammonia_public.xlsx

[45] 2013/14 benchmark. IPPC BAT Ref Large Volume Inorganic Chemicals – Ammonia, Acids and Fertilisers, p.38 shows a range of 1,15 – 1,4 tCO_2/tNH_3

$$CH_4 + 0{,}3035\ O_2 + 1{,}131\ N_2 + 1{,}393\ H_2O \quad CO_2 + 2{,}262\ NH_3$$

This entire ammonia synthesis process scheme is characterized by a high level of heat integration and is a net steam exporting process of about 4.3 GJ/t NH_3[46]. CO_2 emissions are at 1.83 tCO_2/tNH_3 including the already mentioned 1.33 t feedstock-related CO_2 generation.

4.2.2 Low-carbon ammonia production (TRL 7)

In principle, low-carbon ammonia synthesis is limited to an alternative, low-carbon hydrogen production, as ammonia itself does not contain carbon. This hydrogen can be provided by water electrolysis. The process scheme is depicted in Figure 6. Compared to the conventional process, primary and secondary reforming, shift converter and acid gas removal (CO_2 capture) can be omitted. On the other hand, an air separation unit is required, as the supply of pure nitrogen due to oxygen consumption of process air in the secondary reformer is not available any more. Hydrogen is provided by water electrolysis Depending on the electrolysis technology, potentially a hydrogen purification step after electrolysis has to be considered. Electrolyser manufacturers indicate hydrogen purities of 99.5% to 99.9998%[28], however ammonia catalyst sensitivity on remaining impurities has to be checked.

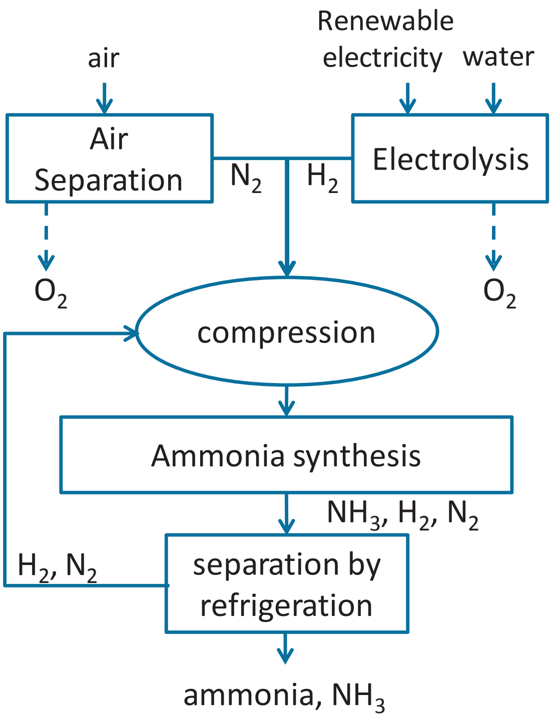

Figure 6: Scheme of low-carbon ammonia synthesis

Compressors are also needed for both hydrogen and nitrogen to compress to the required 100-250 bar for ammonia synthesis as well as for refrigeration. Today pressurised electrolysers, typically deliver hydrogen at 30 bars. Conventional ammonia plants use steam turbines driving the synthesis gas compressor, the air compressors and the refrigeration compressors and require about 3.9-6.5 GJ/t NH_3.

The same order of magnitude is also estimated for low-carbon ammonia production. As the endothermic methane steam reforming is omitted, the amount of required energy and corresponding process related emissions are reduced. On the other hand, no excess steam is

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[46] Industrial Efficiency Technology Database (http://ietd.iipnetwork.org/content/ammonia)

generated in the secondary reformer. Finally, as opposed to conventional ammonia synthesis, no CO_2 is formed as co-product in this synthesis route. The individual technologies are in principle available and the system integration should be relatively straightforward, nevertheless combination of electrolysis with ammonia synthesis is not at commercial stage and a certain level of heat integration will be lost in such a setup.

4.2.3 Energy demand per unit of ammonia production

Water electrolysis is the main energy intensive step in the power-to-ammonia production. Electricity demand for renewable ammonia was estimated at 10 $MWh_{el}/t\ NH_3$ in a study by Öko-Institut[47]. Own calculations indicate an electricity demand for electrolysis of 9.1 MWh or 38.9 GJ (at 4.3 kWh/m^3 hydrogen) to supply the 178 kg hydrogen needed per ton of ammonia.. Additionally, around 1.4 MWh (5 GJ) per t NH_3 are estimated for compressors (see above). For the ASU, 0.4 MWh/tN_2 is assumed[48], corresponding to 0.33 MWh/tNH_3 (1.19 GJ), ending up at a total energy demand of 12.5 MWh or 45.1 GJ per ton of ammonia. In addition, the carbon-free route provides 4.3 GJ/t NH_3 less steam, which has to be provided otherwise. In the scenario work, this is accounted for as part of the electricity-based steam generation in chapter 3.1. For comparison: the energy demand for NG ammonia plants in Europe is 35 GJ, of which 21 GJ correspond to feedstock consumption, resulting in an average SEC around 14 GJ/tNH_3. Energy demand of the low-carbon ammonia process is therefore 3.2 times that of the fossil process (feedstock excluded). Table 11 compares the two routes.

Table 11: Comparison of energy demand

per t NH_3	Fossil (SMR+ NH_3 synthesis)	Low carbon (power to NH_3)
Energy feedstock [GJ]	21	-
Fuel demand [GJ]	10.9	-
Electricity [GJ]	0.74	38.9
Compressors	5	5
Other utilities	1.7 (aux. boiler, flare etc.)	1.19 (ASU)
Steam balance [GJ]	-4.3	0
Total energy demand [GJ] **(SEC [GJ]**	35.04 (14 excl. feedstock)	45.1 (49.4 incl. compensation for

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[47] H. Hermann, L. Emele, C. Loreck, Prüfung der klimapolitischen Konsistenz und der Kosten von Methanisierungsstrategien, p. 25-26, Berlin, 2014; retrieved 11 Sept. 2015, http://www.oeko.de/oekodoc/2005/2014-021-de.pdf.

[48] M. Matzen, M. Alhajji, Y. Demirel, Technoeconomics and Sustainability of Renewable Methanol and Ammonia Productions Using Wind Power-based Hydrogen; J Adv Chem Eng 2015, 5,128, doi:10.4172/2090-4568.1000128

		the missing steam export)
Feedstock related CO_2 emissions [t]	1.33	-
Process emissions [t]	0.5	0.12
Total emissions [t]	1.83	0.12

4.2.4 CO_2 reduction per unit of ammonia production

Table 11 also compares the CO_2 emissions of the two routes. Total CO_2 emissions of the natural gas based ammonia synthesis are at 1.83 tCO_2/tNH_3, of which 1.33 tons are feedstock-related CO_2 emissions, the rest is accounted for by the process related fuel (55.9 $kgCO_2eq/GJ$ NG) and electricity consumption. The low-carbon pathways comprises only process energy related emissions. It is assumed that the process is exclusively based on low-carbon electricity for the supply of hydrogen, but also for supplying heat as steam for compressors and for the ASU. At this point it has to be emphasized again, that all hydrogen-based technologies described in this study only achieve a positive GHG impact, if low-carbon electricity is used.

Based on this assumption, the carbon footprint of electricity and hydrogen production as stated in chapter 4.1.1.5 have been used for calculation of the process carbon footprint. The total footprint is at 0.12 $tCO2eq/tNH_3$, 0.1 tCO_2eq/tNH_3 accounting for electrolysis and the remaining emissions for additional steam generation. The missing excess steam as compared to the SMR process is included in the steam generation in chapter 3.1.

As a result, replacing a ton of ammonia from natural gas as feedstock for the hydrogen supply, this accounts for 1.71 t avoided CO_2.

4.2.4 Economics of low-carbon ammonia production

Given the energy demand of low-carbon ammonia production, the electricity costs per ton of ammonia would be 626 € at 50 €/MWh electricity costs. Adding capital and operating expenses, the costs will rise to 800 €. The fuel costs per ton of ammonia from natural gas are at 35 € to 45 €, compared to the average 600 € using the electrolysis pathway. [49] A plant concept developed by Leighty et al. estimated capital costs associated with ammonia synthesis equipment (including an air separation unit but excluding tank storage and transportation) for an electrolytic ammonia synthesis of 940 € per kW of electricity input. Assuming a cost recovery factor of 12 percent, an ammonia synthesis plant with 100 MW of electricity capacity producing about 73,000 tons of ammonia/year would provide one metric ton

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[49] J. H. Holbrook, W. C. Leighty, Renewable Fuels: Manufacturing Ammonia from Hydropower, Hydro Review 28 (7). accessed on 10 September 2014 at http://www.hydroworld.com/articles/hr/print/volume-28/issue-7/articles/renewable-fuels-manufacturing.html

of ammonia for 735-800 € at 50 €/MWh and 255 -380€ at 10 €/MWh.[50]

Table 12: Low.carbon ammonia production costs

Low-carbon electricity price [€/MWh]	10	30	50
Ammonia production costs [€/t] (continuous operation assumed)	255-380	450-590	735-800
Cost ratio low-carbon/fossil ammonia	1.7-2.5	3-3.9	4.9-5.3

Manufacturing costs of renewable ammonia therefore strongly depend on the price of low-carbon electricity, as shown in Table 12, and very low prices are a prerequisite match the market prices for “conventional” ammonia. Natural gas based ammonia production costs in Europe have been quantified at 350 €/tNH_3[51]. Hydrogen based ammonia production will therefore be competitive only at extremely low electricity prices. The same is true for urea production (chapter 4.3), as it builds on ammonia as feedstock.

4.2.5 Hybrid ammonia production

One drawback of the described low-carbon route is the need of both an electrolyser and an air separation unit, two capital intensive unit operations. In a natural gas plant, air can be used instead of pure nitrogen, as the oxygen is consumed in the secondary reformer. In a transition phase, a **hybrid plant concept** might be an option, in which natural gas is still used as a second feedstock and a reformer section is included. This would allow for a flexible operation of the electrolyser and maintain the high level of process and heat integration of today’s ammonia plants. In addition, CO_2 generated in the reformer can directly be used in subsequent urea production (chapter 4.3). Such a concept has been described by Schulte-Beerbühl[52]: Table 13 summarizes the pros and cons of the pure electrolysis vs. the hybrid concept.

Table 13: Comparison of electrolysis vs. hybrid ammonia and urea plants

	Electrolysis-based	Hybrid
Pro	• Fossil feedstocks avoided	• CO_2 source integrated for urea production • ASU avoided • Process integration maintained

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[50] Ranges adopted from Ref. 33.

[51] A. Boulamanti, J. A. Moya, Production costs of the chemical industry in the EU and other countries: Ammonia, methanol and light olefins; Renewable and Sustainable Energy Reviews, 2016, http://dx.doi.org/10.1016/j.rser.2016.02.021.

[52] S. Schulte-Beerbühl: Herstellung von Ammoniak unter Berücksichtigung fluktuierender Elektrizitatspreise, PhD thesis 2014.

		• Flexibility in operation
Con	• Air separation unit needed (CAPEX) • Continuous operation needs to be ensured • CO_2 import logistics • Process integration lost	• Not fossil-free • No CO_2 recycling • Higher CO_2 emissions, as fossil feedstocks are used

4.3 Downstream production of urea from low-carbon ammonia and CO_2

Urea is widely used in fertilizers, but is also a building block for urea-formaldehyde and urea-melamine-formaldehyde resins. In Europe, urea is produced at 6 Mt p.a.[53]

Urea production is often highly integrated with ammonia plants, as the CO_2 produced by the reforming process and recovered from the flue gas of the reformer or boiler are fed together to the urea synthesis section as feedstock. For this reason urea has been added to the target products in this study. The ammonia and carbon dioxide are fed into the urea reactor at high pressure and temperature, and the urea is formed in a two step reaction. Unreacted NH_3 and CO_2 are recycled.

Ammonium carbamate synthesis: $2\ NH_3 + CO_2 \rightarrow NH_2COONH_4$ $\Delta H^0 = -159.7$ kJ/mol

Urea synthesis: $NH_2COONH_4 \rightarrow H_2O + NH_2CONH_2$ $\Delta H^0 = +41.43$ kJ/mol

In case ammonia is produced via the low-carbon route, CO_2 is not generated in a reformer step and needs to be imported from other sources. This is the first process in this chapter in which recycling of CO_2 is enabled. Captured CO_2 from fossil fired power plants or industrial processes can be used for CO_2 supply.

4.3.1 Energy demand and CO_2 reduction per unit of urea production

The energy demand of an isolated urea production is difficult to estimate, as this process is usually highly integrated in the ammonia production plant. As a literature reference[54] additional 3.29 GJ/turea for production of steam otherwise provided by excess steam in the ammonia plant is estimated. Corresponding CO_2 emissions have been estimated at 0.32 t CO_2/t urea.[55]
CO_2 is built in a stoichiometric ratio of 1:1 with ammonia into urea. 0.73 t CO_2 per t urea are required, counted as a negative emission (see Figure 1 in chapter 1.4).[29] However, the carbon footprint of the CO_2 supply has to be taken into account, see Box 1. For the CO_2 demand of

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[53] IFA, http://www.fertilizer.org/en/doc_library/Statistics/PIT/urea_public.xlsx

[54] http://www.thyssenkrupp-industrial-solutions.com/fileadmin/documents/publications/ Nitrogen-Syngas-2011/Low_Energy_Consumption_Ammonia_Production_2011_paper.pdf

[55] J. Fugice et al., International Fertilizer Development Center (IFDC) Muscle Shoals, Alabama; https://dl.sciencesocieties.org/publications/meetings/download/pdf/2015am/93574

urea production, 0.31 t CO_2/t urea of indirect emissions have to be taken into account. The total CO_2 footprint would therefore amount to -0.42 t per t urea.

Box 1: **Carbon Footprint of CO_2 as a feedstock for chemical processes**

CO_2 used as feedstock is a relevant process input flow. System boundaries of an LCA should therefore include all upstream processes of feedstock CO_2 starting at the CO_2 source.[56]

CO_2 capture requires energy, but also additional equipment and working materials such as capture solvents. Furthermore, the captured CO_2 is usually compressed and needs to be transported. All these contributions lead to indirect CO_2 emissions that need to be included in the carbon footprint of CO_2 as feedstock. The actual amount of indirect emissions depends on factors such as:

- quality of the source, i.e. industrial plant or power plant source, CO_2 concentration and purity;
- capture process, i.e. efficiency and energy requirement/penalty as well as further CO_2 purification needs
- transport logistics, i.e. the geographic distance between CO_2 source and chemical production site.

An in-depth analysis of these different factors and their sensitivity is out of scope of this study. For assessment of the carbon footprint of the CO_2 source, CO_2 capture, compression and transport from a power plant have been taken from reference 57, which is at approximately 0.42 t CO_2 per ton of CO_2 captured. This value represents a relatively conservative rather than an ideal case, as other industrial sources provide higher CO_2 concentrations. More information on this is provided in the Annex.

To reflect the entire process chain from water and CO_2 via ammonia to urea, the energy demand and carbon footprint of the ammonia required as feedstock have to be included. As 0.57 t ammonia are required per ton of urea, this accounts for 25.7 GJ (7.1 MWh) per t urea and 0.07 tCO_2/t urea as additional energy demand or CO_2 emissions respectively. Total energy consumption would therefore be at 29 GJ (8.1 MWh) per t urea, and the CO_2 footprint at -0.35 tCO_2/t urea. Emissions of the fossil urea production are at 1.7 tCO_2/t urea.[58] Avoided CO_2 compared to the fossil route would then correspond to 2.05 tCO_2/t urea.

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[56] N. von der Assen, P. Voll, M. Peters, A. Bardow: Life cycle assessment of CO2 capture and utilization: a tutorial review; Chem. Soc. Rev., 2014, 43, 7982-7994.

[57] Niklas von der Assen, Johannes Jung and Andre Bardow: Life-cycle assessment of carbon dioxide capture and utilization: avoiding the pitfalls; Energy Environ. Sci., 2013, 6, 2721-2734.

[58] J. Fugice, U. Singh, D. Hellums, Urea for CO_2 Fertilization, International Fertilizer Development Center (IFDC) Muscle Shoals, Alabama; https://dl.sciencesocieties.org/publications/meetings/download/pdf/2015am/93574

4.3.2 Economy of low-carbon urea production

Taking the cost range for ammonia production of 700-800 €/t and the feedstock of urea, 0.57 t ammonia, 450-500€ are estimated as the production costs of low-carbon urea.

4.4 Methanol production from hydrogen and CO_2

Methanol is one of the largest volume chemicals in the world and serves as source for various other compounds. Amongst those, formaldehyde is the one with the largest production volume; it accounts for 30% of the worldwide methanol demand, other important products are methyl-tert-butyl ether (MTBE) and acetic acid. In Europe, methanol is predominately produced from natural gas via steam reforming, to a very small extent also from heavy oil. Production volume is at 1.5 million tons. For the traditional use of methanol, i.e. not considering additional demands based on the technologies described in this study, production is expected to increase to 2.17 million tons in 2050[59].

Future development of methanol production will depend on different factors, such as the development of the oil price.

4.4.1 Conventional methanol production (TRL 9)

Up to date methanol is quasi exclusively produced in large scale plants up to 3000 tpd capacity from synthesis gas, which again is generated by reforming of natural gas. One can produce methanol from CO as well as from CO_2, whereas in the production from CO_2, a water-gas shift step needs to be included to remove excess CO_2 from the feed-gas stream.

CO Hydrogenation: $CO + 2\,H_2 \rightarrow CH_3OH$ $\Delta H^0 = -90.8$ kJ/mol

CO_2 Hydrogenation: $CO_2 + 3\,H_2 \rightarrow CH_3OH + H_2O$ $\Delta H^0 = -49.5$ kJ/mol

emissions are at 0.52 tons per ton of methanol for natural gasl[60].

The general process scheme can be described in a simplified manner as follows: after feed purification, mainly desulphurization, the feed is pre-heated and steam is added to the natural gas. The mixture is fed into the reformer at 20 bar pressure, in which hydrogen and carbon monoxide (syngas) and around 5% CO_2 (with also some remaining residue methane) are formed in the catalytic steam reforming reaction at 800-950°C. The process gas is cooled in a process boiler, producing steam for the process and excess steam, which can be exported. A high level of heat integration is ensured. Some CO_2 is added to the feed gas to adjust the syngas to have the ideal ratio to efficiently produce methanol.

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[59] Prodcom data and assumed 1% p.a. increase

[60] Technology Roadmap "Energy and GHG Reductions in the Chemical Industry via Catalytic Processes - Annexes; IEA/ICCA DECHEMA, 2013.

For the subsequent methanol synthesis, a large variety of reactor designs is available from different licensors, the technology is therefore described in general terms. The syngas is compressed and fed into the methanol converter. Methanol conversion is at approximately 5% per pass, hence unreacted gases are recycled in the synthesis loop. The converter design affects the loop pressure. The synthesis loop comprises a circulator and converter. Reaction heat from the loop is recovered as steam. A purge from the synthesis loop is taken to continuously remove inert gases accumulated during the recycle loops and sent to the reformer section. The crude product contains water and traces of byproducts. Nonreacted gases are removed in a separator and methanol is separated from water by distillation. The SEC of the methanol process in Europe is at 12.5 GJ/t methanol, which mainly comprises fuel in the reformer, with 0.6 GJ/t of electricity use. BPT level is around 9.8 GJ/t.[6] Sufficient heat is produced in the process to run the methanol distillation, in fact, methanol production is a net steam exporter of around 2 GJ/t methanol.

4.4.2 Low-carbon methanol production (TRL 7)

The alternative low-carbon pathway to methanol is again based on hydrogen, produced by water electrolysis with low-carbon electricity followed by hydrogenation of CO_2 as carbon source.

Electrolysis: $6\ H_2O + \text{electrical energy}_{(\text{wind/solar})} \rightarrow 6\ H_2\ (\text{cathode}) + 3\ O_2\ (\text{anode})$

Hydrogenation: $2\ CO_2 + 6\ H_2 \rightleftharpoons 2\ CH_3OH + 2\ H_2O \quad \Delta H_{298K,\ 50\ bar} = -40.9\ kJ/mol$

Total: $2\ CO_2 + 6\ H_2 + \text{electrical energy}_{(\text{wind/solar})} \rightarrow 2\ CH_3OH + 2\ H_2O + 3\ O_2$

Hydrogenation of CO_2 is used also in conventional methanol production by adding small amounts of CO_2 to adjust the CO/H_2 ratio of the syngas. Synthesis of methanol from CO and CO_2 are tied through the water gas shift reaction.

Water gas shift: $CO + H_2O \rightarrow CO_2 + H_2 \qquad \Delta H^0 = -41.2\ kJ/mol$

The anticipated direct synthesis of methanol from CO_2 does not use a „Reverse Water Gas Shift (RWGS)“ reactor, in which CO_2 is reduced to CO by hydrogen, to yield classical CO/H_2 synthesis gas for methanol synthesis.

For the hydrogenation of pure CO_2 to methanol, catalysts are commercially available, and a number of pilot plants are in operation, e.g. by Mitsui Chemicals (Japan) and Carbon Recycling International (Iceland, see Box 2) to investigate the feasibility of industrial-scale production. CO_2 hydrogenation to methanol is accompanied by water formation, and the recycle gas and crude methanol contain much more water compared to the conventional process, which has to be removed by distillation. Figure 7 shows a general process scheme, in which CO_2 originates from a coal fired power plant. As renewable electricity depicted in the scheme is not continuously available, a temporary storage of hydrogen is foreseen to allow for steady-state operation of the methanol reactor. As in the low-carbon ammonia production, the electrolysis potentially needs to be followed by a hydrogen purification step and compression.

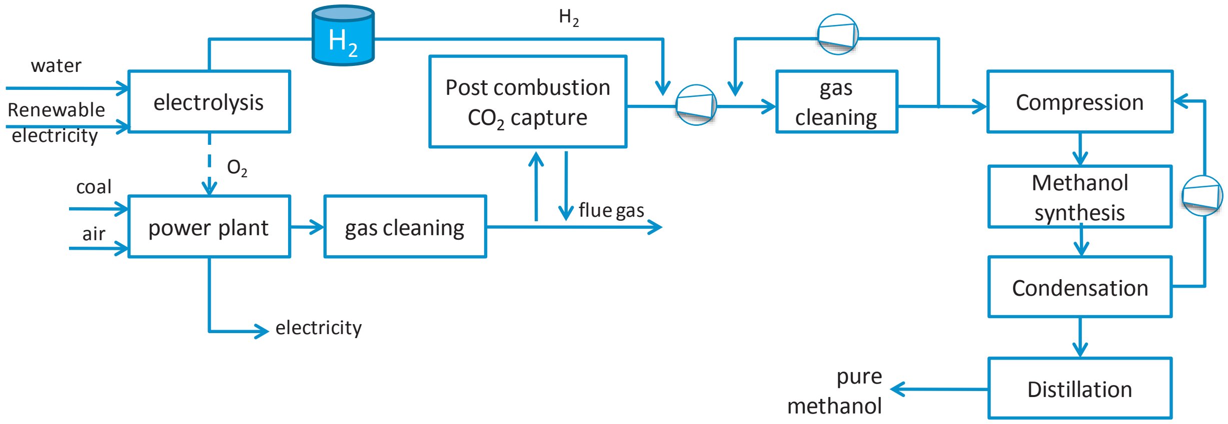

Figure 7: Power to methanol scheme using renewable electricity

Alternative concepts to produce conventional CO/H_2-syngas are in an early development phase and include direct electrochemical reduction of CO_2 and electrocatalytic co-reduction of CO_2 to CO and water to hydrogen. These concepts are investigated in a number of research institutes on lab-scale, their TRLs are therefore relatively low (TRL 1-3).

Box 2: **Renewable Methanol Pilot Project in Iceland**

In 2011, Carbon Recycling International (CRI) started operation of the "George Olah Renewable Methanol Plant" and hereby demonstrated the potential of tapping into Iceland's geothermal energy. The 7.1 € million plant (for a capacity of 1,300 metric tons) was designed to currently produce 4000 tons of renewable methanol per year (5 million liters). This plant serves as a pilot study for the planned extension to a 40.000 tons plant. The feed consists of CO_2 from geothermal power plant and hydrogen produced by 5 MW water electrolysis fed by a geothermal power plant. All units are operated continuously. The methanol product is mixed into gasoline and substitutes up to 2.5% of Iceland's fuel consumption. Further uses are as feed in biodiesel production or in other methanol-based processes. In comparison to fossil-fuel based methanol, renewable methanol reduces GHG emissions by 90%.

4.4.3 Energy demand per unit of methanol production

As in ammonia synthesis, water electrolysis is also the main energy intensive step in the power-to-methanol production chain. Assuming 4.3 kWh/m^3 hydrogen as energy demand for water electrolysis, 9.52 MWh$_{el}$ (34.3 GJ) are required for producing the 189 kg hydrogen stoichiometrically needed per ton of methanol according to own calculations. Another study quantified 9.2 MWh_{el} / t methanol.[61].

Approximately 1.5 MWh/t (5.4 GJ) are additionally required for utilities (compressor, distillation)[62] resulting in 11.02 MWh/ t (39.7 GJ) methanol in total. The net steam export of the conventional methanol process is not realized in the low-carbon process route. This has to be provided otherwise. In the scenario work, this is accounted for as part of the electricity-based steam generation in chapter 3.1. The total energy demand of the low-carbon process is substantially higher than for the conventional route (factor 3). However, the difference is less pronounced, if the feedstock is included in the energy demand of the fossil process. It has to be emphasized, that all hydrogen and CO_2-based processes generate the target molecules from the end of pipe products water and CO_2, whereas the fossil routes benefit from the energy content of the employed fossil feedstock. If replacing fossil feedstocks is a general goal, the energy content of the target products is part of the energy demand of the process. Table 14 compares the conventional with the low-carbon methanol route.

Table 14: Comparison of energy demand and CO_2 emissions for methanol production routes

per t methanol	Fossil (SMR+ methanol synthesis)	Low carbon (power to methanol)
Energy feedstock [GJ]	25	-
Fuel demand [GJ]	13.9	-
Electricity [GJ]	0.6	34.3
Utilities [GJ]		5.4
Steam balance [GJ]	-2	0
Total energy [GJ]	37.5 (12.5 excl. feedstock)	39.7 (41.7 incl. compensation for missing steam export)
Feedstock related CO_2 emissions [t] [63]	0.97	-0.79
Process emissions [t][63]	0.52	0.123
Total emissions [t] [63]	1.49 (1.82 cradle to gate)	-0.67

4.4.4 CO_2 reduction per unit of methanol production

The CO_2 footprint of the low-carbon methanol synthesis comprises two contributions: i. the consumption of CO_2 as carbon feedstock and ii. the process related emissions, in this case predominately or exclusively caused by electricity, the latter in the case a full electrified

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[61] H. Hermann, L. Emele, C. Loreck, Prüfung der klimapolitischen Konsistenz und der Kosten von Methanisierungsstrategien, p. 27, Berlin, 2014.

[62] Personal communication

[63] see following chapter 4.4.4

concept including steam generation is enabled. Stoichiometrically, 1.373 t CO_2 are required per ton of methanol for the synthesis. As described in chapter 1.4 and Box 1, the feedstock CO_2 is accounted for as negative emissions, but reduced by the carbon footprint of the CO_2 supply. For the CO_2 demand of methanol, 0.58 t CO_2/t methanol of indirect emissions have to be taken into account, reducing the amount of avoided CO_2 to 0.79 t CO_2/t methanol. The process related emissions calculated according to the methodology described in chapter 4.1.1.6 are at 0.123 tCO_2eq/t methanol, 0.106 t accounting for hydrogen production and 0.017 t for the remaining required process energy. The missing excess steam as compared to the SMR process is included in the steam generation in chapter 3.1. The total footprint of the low-carbon methanol process is therefore at -0.67 tCO_2/t methanol. The NG based process has a footprint of 0.52 tCO_2/t methanol6 and 0.85 tCO_2/t methanol cradle to gate, i.e. including the upstream emissions of natural gas (production and transport).[64]

As a result, replacing one ton of methanol from natural gas as feedstock by the low-carbon methanol accounts for 1.53 t avoided CO_2.

4.4.5 Economics of low-carbon methanol production

A comparison of a low-carbon power to methanol plant with a low-carbon power to SNG plant has been provided by Plass et.al[65]. The comparison shows that production costs (CAPEX +OPEX) for methanol and SNG, expressed as € per GJ, are very similar. Absolute values depend on the operating hours per year, a measure which accounts for the non-steady availability of wind or solar power, and of course the costs of renewable electricity. At an operating time of 7000 h/year, methanol production costs are at 670 €/t for 50 €/MWh power cost, an operation time of 3000 h/year would result in 826 €/t. Another study calculates today's costs of "green methanol" production at 600 €/t [66]. Table 15 shows that the costs of methanol strongly depend on the price of renewable electricity.

Table 15: Costs of production for renewable methanol assuming different hours of operation[67]

Renewable electricity price [€/MWh]		10	30	50
Methanol production costs [€/t]	at 7000 h/year	290	469	670
	at 5000 h/year	335	536	737
	at 3000 h/year	447	625	826

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[64] 14.7kgCO_2/GJ NG according to ICF Consulting Canady, Life Cycle Greenhouse Gas Emissions of Natural Gas, 2012; calculation: 14.7kg/GJ x 45.1 GJ/t x 0.5 tNG/tMeOH = 0.331 tCO_2/t MeOH

[65] M. Bertau, H. Offermanns, L. Plass, F. Schmidt, H.-J. Wernicke (Eds.), Methanol: The Basic Chemical and Energy Feedstock in the Future, chpt. 8, p. 650.

[66] A. Heberle, E. Kakaras, Mitsubishi Hitachi Power Systems Europe: German Energiewende as Driving Force for New Technologies - Power Industry meets Process Industry, presentation at Energy, Science & Technology 2015, 21 May 2015, Karlsruhe, Germany.

[67] Adopted from reference 22.

A recent calculation of production costs for petrochemicals in Europe, provided by the Joint Research Centre of the European Commission amounted to 400 €/t methanol[51]. Other sources quantify the span of worldwide production costs of methanol based on fossil feedstocks between 60 and 260 €/t[68]. The high volatility of feedstock costs makes projections and hence a reliable margin for investment decisions very difficult. It has to be concluded that 100% renewable energy based methanol hardly provides a business case without subsidies, even under ideal conditions (high level of operating hours and low renewable electricity price).

The electrolysers represent 75% of the total installed costs and therefore predominate the capital costs. Hence, reduction of electrolyser costs is key to further reduce overall production costs. In the example above, reducing alkaline electrolyser costs from 1000-1200 to 500-700 €/kW, anticipating realistic technology improvements, would result in 50% reduced capital costs and about 30% lower total costs for methanol production. Major cost reductions by economy of scale effects are not to be expected, as electrolyser capacity is mainly increased by numbering up of stacks.

4.5 Ethylene and propylene via hydrogen-based methanol (TRL 8-9)

Ethylene and propylene are large scale petrochemical products and primary building blocks of the chemical tree opening up synthesis pathways for many other large scale products including polyethylene and polypropylene, styrene (via ethylbenzene), monoethylene glycol (via ethylene oxide), acrylic acid, acrylonitrile, cumene and polyols (via propylene oxide), just to name some of the most important. Ethylene is produced at 21.7 Mt p.a. in Europe, propylene at 17 Mt.

4.5.1 Conventional ethylene and propylene production (TRL 9)

Production of ethylene and propylene in Europe is mainly performed by steam cracking with Naphtha as the predominate feedstock, although Liquefied Petroleum Gas (LPG) is gaining importance in Europe, and 25% of feedstock used in the steam crackers in 2015 was LPG.[69]. Usually crackers can use a mix of feedstock, and very few crackers would use LPG only. Along with ethylene and propylene steam cracking also yields other products, together referred to as high value chemicals (HVC).[70]

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[68] D. Johnson, Global Methanol Market Review, IHS 2012, http://www.ptq.pemex.com/productosyservicios/eventosdescargas/Documents/Foro%20PEMEX%20Petroqu%C3%ADmica/2012/PEMEX_DJohnson.pdf

[69] https://www.gep.com/mind/blog/rise-lpg-petrochemical-feedstock-asia-and-europe

[70] HVC (high-value chemicals) refers to products from naphtha cracking. This process delivers ethylene and propylene as main products, but also forms a number of other valuable by-products. Hence, energy consumption is allocated to the whole range of HVC products.

The process starts with mixing the feedstock with steam and heating in furnaces to 750 °C–900 °C, where naphtha is cracked into products of lower chain length. The cracked gas is subsequently cooled down, thereby recovering the heat as steam. Benzene, toluene, xylene are separated at around 150°C, water is removed and the remaining gas is compressed, followed by fractionation of the gas into the different products. Methane is recycled as fuel into the furnace. A higher cracking severity favours ethylene production whereas lower severity yields higher amounts of propylene. The SEC of Naphtha-based steam cracking in Europe is around 16.5 GJ/t HVC, the value for BPT plants is around 12 GJ/tHVC.[6]

4.5.2 Low-carbon production of ethylene and propylene via MTO (TRL8-9)

In contrast to the previously described processes, there is currently no existing process at an advanced TRL, which directly uses hydrogen and CO_2 to produce olefins. Current research efforts such as the project eEthylene under the lead of Siemens[71], funded by the German Ministry of Education and Research, aim at a direct electrocatalytic production of ethylene from CO_2 and water in a single stage system. While the general proof of concept has been shown, this technology is still at TRL 3-4. Nevertheless this technology could be a breakthrough, as it omits the need of intermediate products such as methane or methanol as feedstock for olefin synthesis. The production pathway included herein is based on the previously described methanol production from hydrogen and CO_2 followed by the methanol to olefin process, which is currently commercially deployed, albeit commercial operations are located in China and no MTO plant is operated in Europe so far. The process sequence is depicted in Figure 8.

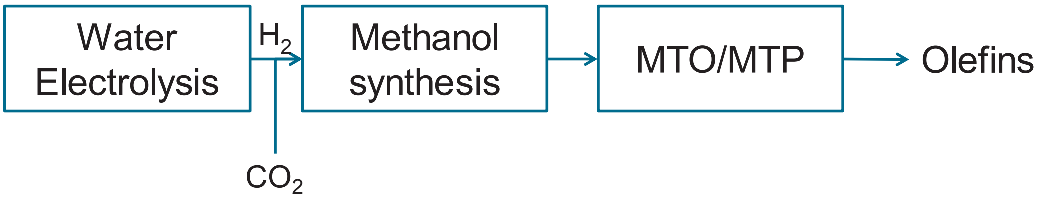

Figure 8: Low-carbon process sequence to ethylene and propylene via methanol

Different processes are licensed, such as the UOP/Hydro MTO technology based on the MTO-100 silicoaluminophosphate synthetic molecular sieve based catalyst, and Lurgi's MTP (methanol-to-propylene) process based on MTPROP, a proprietary ZSM-5 type of catalyst supplied from Clariant (former Süd-Chemie).

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[71] https://www.siemens.com/innovation/en/home/pictures-of-the-future/research-and-management/materials-science-and-processing-eethylen.html

The MTO reaction is strongly exothermic. To control the heat of reaction and the adiabatic temperature increase, the process follows a two-step dehydration of methanol to DME and water, followed by the conversion to olefins, as depicted in the following reaction equations:

$2\ CH_3OH \rightarrow CH_3OCH_3 + H_2O$
$CH_3OCH_3 \rightarrow C_2H_4 + H_2O$
$3\ CH_3OCH_3 \rightarrow 2\ C_3H_6 + 3\ H_2O$

Depending on the catalyst, different target products can be realized subsequently, besides MTO the methanol-to propylene (MTP) process, or methanol to gasoline (MTG) process shall be mentioned. The two major process concepts are based on a fixed-bed and a fluidized-bed reactor.

Based on fossil feedstock, and NG specifically, the process sequence would accordingly start with steam reforming and methanol production, followed by MTO. BPT energy consumption of MTO plants are at 5 GJ/tHVC[72]. Assuming BPT level for plants in Europe seems reasonable, as currently no MTO production capacities exist and new plants would have to be built. In addition, the energy consumption for producing methanol as feedstock has to be included in the total energy consumption of the process chain, resulting in 17.5 GJ/tHVC, which is above steam cracking. In terms of CO_2 emissions, the process sequence of NG to olefins via MTO would not be beneficial, as steam cracking emits 0.76 tCO_2/tHVC compared to 2.9 tCO_2/tHVC for the process chain via MTO. The latter includes 0.5 tCO_2/tHVC[6] for MTO plus the emissions caused by production of 2.83 t methanol stoichiometrically required as feed in the MTO process.

For the low-carbon route, the MTO process would remain unmodified, emission reduction is then predominately based on providing low-carbon methanol as feedstock.

4.5.3 Energy demand per unit of ethylene/propylene production via methanol

Stoichiometrically, 2.28 tons of methanol are required per ton of ethylene or propylene. Energy demand therefore is composed of the energy demand for hydrogen-based methanol production as described in chapter 4.4.2 and the energy demand for the MTO process, which is at 5 GJ/t HVC. In total energy demand is at 95.5 GJ/t HVC corresponding to 26.6 MWh/t HVC, based on electricity. This is more than 5 times the energy demand of the naphtha based process (16.5 GJ/t HVC). Even if the feedstock energy content (42.5 GJ/tHVC) is taken into account for steam cracking, the SEC of the low-carbon process is still 40% higher. It has to mentioned also, that Naptha steam cracking is a net steam exporting process (1.5 GJ/tHVC), this is accounted for under electricity-based steam generation (see chapter 3.1).

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[72] IEA expert consultation

4.5.4 CO_2 reduction per unit of ethylene/propylene production

The MTO process causes 0.4 t CO_2eq/t HVC[73] compared to 0.76 tCO_2eq/t HVC[6] in the naphtha-based process. The main benefit of the low-carbon process sequence in terms of CO_2 emissions would however originate from the low-carbon methanol production, as this process has been shown to be a net CO_2 consuming process (negative emissions). The process sequence would therefore benefit from the strong methanol demand of the MTO process, which on the other hand causes the very high energy consumption indicated above. Taking the CO_2 feedstock demand and footprint for the hydrogen-based methanol production into account, the total carbon footprint of the process chain from water and captured CO_2 to methanol and further to olefins amounts **to -1.89 t,** which is the avoided CO_2 per ton of ethylene or propylene produced via this pathway.

For the scenario work, it is assumed, that a share of new olefin production plants corresponding to the projected increase in production volumes is to be realized as the process chain of hydrogen-based methanol production followed by MTO. In addition, it is assumed that the continuous replacement or retrofit of old plants will be partially based on this route.

4.5.5 Economics of low-carbon ethylene and propylene production

Economic constraints described in the methanol chapter remain an issue also for the olefin production, as methanol is the feedstock. For methanol production costs between 300 and 650 €/t feedstock costs will amount to 680 to 1450 € per ton of ethylene or propylene. A recent calculation of production costs for ethylene and propylene from Naptha in Europe, provided by the Joint Research Centre of the European Commission[51] amounted to 816 €/t HVC: an economic gap of at least a factor 2 has to be estimated, making the realization of this pathway very challenging, in particular, as new investments in both hydrogen-based methanol plants and MTO plants would be necessary.

4.6 Benzene, toluene and xylenes via hydrogen-based methanol (TRL 7)

Benzene, toluene and xylene (o- and p-xylene) are major aromatic compounds used for the production of synthetic fibers, resins, detergent and polymers, including for instance (poly)styrene, polyurethane and polyesters. BTX are produced at a level of 15.7 mill tons in Europe, with an anticipated growth to 29 million tons in 2050.

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[73] Technology Roadmap "Energy and GHG Reductions in the Chemical Industry via Catalytic Processes - Annexes; IEA/ICCA DECHEMA, 2013.

4.6.1 Conventional production of BTX [TRL9]

BTX production in Europe mainly follows the same pathway as the previously described olefins, i.e. steam cracking of Naphtha. BTX is extracted from pygas, a by-product of high temperature naphtha cracking containing around 65% aromatics. Another process is catalytic reforming of Naphtha yielding high-octane gasoline and BTX rich aromatics. The share of aromatic compounds in Naphtha steam cracking products is around 14%. The SEC of BTX production is at 7 GJ/tHVC.

4.6.2 Low-carbon production of BTX via hydrogen-based methanol [TRL7]

The production pathway considered here is again based on methanol. The process sequence is depicted in Figure 9.

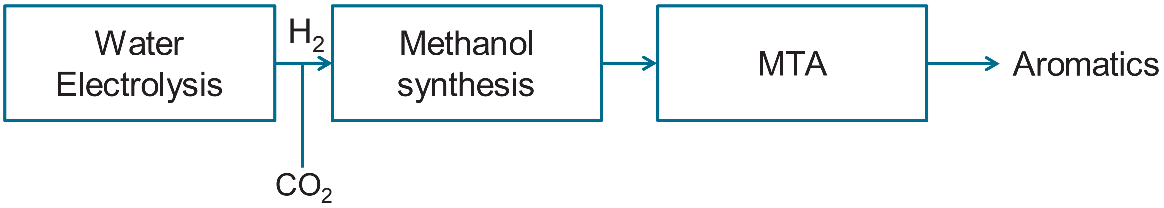

Figure 9: Low-carbon production of BTX via hydrogen-based methanol

Mobil's methanol-to-aromatics (MTA) process has been considered, in which methanol is converted to a range of aromatic compounds using a zeolite catalyst at 370-540 °C and 20 to 25 bar. Compared to the MTO process the temperature is lower and higher catalyst acidity is required. Conversion is at 95 – 100% with an aromatics yield of 60 – 70 % of which 80% are BTX, resulting in a total BTX yield of 56%.[74]

Table 16 shows a typical product spectrum of the MTA process, indicating that on average 7.5 methanol molecules are stoichiometrically required per unit of aromatics produced. Considering the total BTX yield of the process, the methanol demand of the process is 4.3 tons of methanol per ton of BTX.

Table 16: Product spectrum of methanol-to-aromatics (MTA) over HZSM-5[75]

Product	wt%	C atoms	Weighted
Benzene	4.1%	6	0.34
Toluene	25.6%	7	2.51
o-xylene	9.0%	8	1.01
m-Xylene	22.8%	8	2.55

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[74] E. Köhler, Oil, Gas (Hamburg, Ger.) 2014, 2, 70 – 76.

[75] C. D. Chang, Mobil Research and Development Corporation, Catal . Rev.-Sci. Eng. 1983, 25(1). 1-118.

p-Xylene	10.0%	8	1.12
	71.5%		7.53

4.6.3 Energy demand per unit of low-carbon BTX production

Energy demand of the low-carbon production sequence is largely determined by the energy demand of the hydrogen-based methanol production. As 4.3 t/t BTX are required, the energy demand amounts to 171 GJ (or 47.5 TWh) per ton of BTX. The energy demand for the MTA process is assumed to be close to the MTO process, i.e. 5 GJ/t, summing up to 176 GJ/t. This is to be compared to the BTX route from Naphtha, which consumes 7 GJ/t.

4.6.4 CO_2 reduction per unit of low-carbon BTX production

The MTA process emissions are higher than those of the naphtha-based process, i.e. 1.13 t CO_2eq/t BTX compared to 0.55t CO_2eq/t HVC.[73] The major impact is coming from the CO_2 feedstock demand and footprint of the hydrogen-based methanol. The required 4.3 t methanol per t BTX account for -2.91 tCO_2. Taking the production into account, the total carbon footprint of the process chain from water and captured CO_2 to methanol and further to BTX via the MTA process amounts **to -1.7 t,** which is the avoided CO_2 per ton BTX produced via this pathway.

4.6.5 Economics of low-carbon BTX production

As low-carbon methanol is the feedstock for the above described BTX process, the cost of methanol production and resulting feedstock costs largely determine the cost of BTX production. For methanol production costs between 300 and 650 €/t, feedstock costs will amount to 1300 to 2800 € per ton of BTX, if methanol costs are only based on production costs, i.e. without additional margins. Production costs are accordingly extremely high, a factor of 3 and higher is to be expected compared to the incumbent fossil-based technology.

4.7 Synthetic fuels from low-carbon hydrogen and CO_2

As the technologies discussed before can be used to manufacture high quality liquid fuels with low carbon footprint, options for producing synthetic non-fossil fuels for the transport sector have been investigated as part of this study. This becomes more and more important as the need increases to reduce the exhaust of CO_2 generated from fossil sources, the transport sector hereby being one of the largest emitters. The study does not attempt any projections on the role of liquid fuels in the future or how other options such as electromobility or hydrogen as fuel might be deployed. The transportation fuel demand as indicated by the IEA ETP2°C scenario has been used as basis for the later scenario work. In the course of the investigated transition of chemical production towards electricity-based processes, the technologies considered can potentially also be used to produce transportation fuels in the future. Methanol can serve as both chemical raw material and transport fuel or can be used to produce other types of fuels additives or fuels. The Power-to-X technologies can be used to synthesize synthetic fuels from syngas produced from hydrogen and CO_2 via Fischer-Tropsch synthesis. These routes and their potential impact are described subsequently.

4.7.1 Low-carbon methanol as a transport fuel

Methanol has been previously described as a key component for various low-carbon synthesis routes to petrochemicals. However, methanol has also the capability of being utilised as fuel or fuel composite. Methanol can be directly used as high octane liquid fuel and is blended with gasoline and ethanol in today's vehicles at minimal incremental costs. The current European standard, EN 228, as last revised in 2004, allows up to 3% methanol (M3) to be used as gasoline blend. Up to 3 vol% methanol has been proven to have no adverse effects on the engine or material wear. Materials in contact with the fuel may have to be adjusted e.g. to avoid corrosion, phase separation has to be avoided using solubilizers and cold-start and warm-up ability is affected. For very high concentrations, beyond 89 vol% methanol, a hydrocarbon component such as isopentane has to be added for this reason. With a growing rate of more than 24% from 2008 to 2013 the usage of methanol as gasoline blending or for combustion, this usage has become the second largest field[76]. Blends of methanol and gasoline are particularly prevalent in China, from 15 to more than 85 vol.%. Even though the energy density of methanol is considerably lower than gasoline or diesel, the loss in energy storage capacity can be partially offset by the higher energy output generated in the combustion of methanol.

Furthermore, methanol can be used to produce fuel additives including MTBE and tertiary-amyl-methyl ether (TAME). Finally, the Methanol-to-gasoline (MTG) process discovered in the early 1970s allows the production of high-quality gasoline from methanol[77].

4.7.1.1 CO_2 reduction for (partially) replacing gasoline by methanol

For a comparison of carbon footprints of fuels, the whole lifecycle of a given fuel has to be taken into account. CO_2 footprints are therefore compared on the basis of well-to-wheel data. For gasoline, CO_2 emissions well-to-wheel amount to 87,1 g CO_2/MJ.[78] In the case of low-carbon methanol, GHGenius has conducted a LCA for wind-power-based methanol used as fuel resulting in 14g CO_2/MJ well to wheel.[79] In total, this corresponds to a reduction of 73.1 g CO_2/MJ of fuel.

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[76] http://www.methanolmsa.com (retrieved 27/08/2015)

[77] For an overview see M. Bertau, H. Offermann, L. Plass, F. Schmidt, H.-J. Wernicke (Eds) Methanol: The Basic Chemical and Energy Feedstock of the Future, chpt. 6.4.1, p. 440.

[78] WELL-TO-WHEELS Report Version 4.a, Joint Research Centre 2014

[79] http://bluefuelenergy.com/ghgenius/ 10/09/2015)

In the scenario work, methanol is considered as fuel (additive) and a certain share of methanol in gasoline is anticipated. Gasoline demand has been taken from the IEA 2DS ETP2015 Transport model. Additional methanol production capacities are required to meet the demand depicted in the respective scenarios. Table 17 summarizes the impact of using methanol as fuel in different mixtures with gasoline.

Table 17. Impact of methanol as fuel additive in gasoline

Share methanol	0%	5%	10%	25%	50%	60%	80%	100%
Energy density MJ per liter fuel [a)]	32.40	31.56	30.72	28.20	24.00	22.32	18.96	15.60
European gasoline demand [PJ] [b)]	4348	3155	2752	2410	2061	1634	1186	994
Gasoline required [mill. t] [a), b)]	98	68	56	41	23	15	5	0
Methanol required [mill. t] [a), b)]	0	8	14	30	52	49	48	50
Factor more fuel required [c)]	1.00	1.03	1.05	1.15	1.35	1.45	1.71	2.08
Correp. CO_2 emissions [kg/l] [d)]	2.822	2.692	2.562	2.171	1.520	1.260	0.739	0.218
Emission reduction (%)	0%	5%	9%	23%	46%	55%	74%	92%

a) 32.4 MJ/L or 44.4 GJ/t for gasoline, 15.6 MJ/L or 19.9 GJ/t for methanol
b) IEA ETP Transport 2015, 2°C scenario
c) Based on energy density of the fuel mix, higher combustion efficiency of MeOH neglected
d) Emissions well to wheel: gasoline 87,1 g/MJ , methanol 14 g/MJ

4.7.1.2 Economics of low-carbon methanol as fuel

Low-carbon methanol production costs between 300 and 650 €/t would correspond to a range of 1.5 to 3.3 €ct/MJ This would be competitive to bioethanol production costs at 1.5 to 2.5 €ct/MJ, but is a factor 2 above conventional gasoline production.

4.7.2 Production of synthetic diesel and kerosene via hydrogen-based syngas and Fischer Tropsch synthesis (TRL 5-7)

Synthetic gas (syngas) produced from electricity-based hydrogen and CO_2 can be used in Fischer-Tropsch synthesis for the production of various synthetic fuels. The general process scheme is shown in Figure 10.

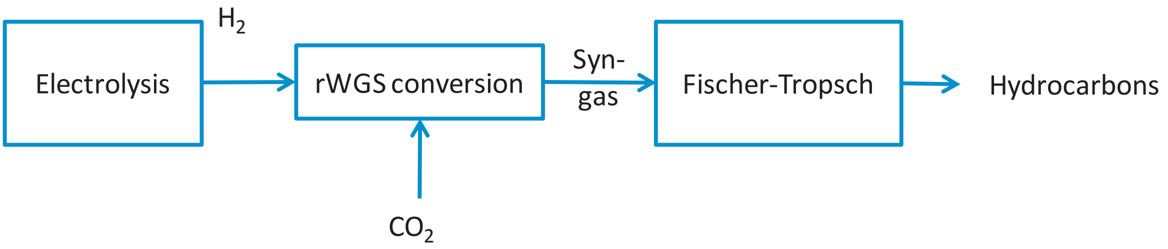

Figure 10: Power to FT hydrocarbons process scheme

The simplified reaction sequence is as follows:

Electrolysis:	$3\ H_2O + e- \text{-->} 3\ H_2 + 1{,}5\ O_2$
Rewerse water gas shift:	$CO_2 + 3\ H_2 \text{-->} CO + 2H_2 + H_2O$
Fischer Tropsch synthesis:	$CO + 2\ H_2 \text{-->} \text{-}CH_2\text{-} + H_2O$

There are several concepts at TRLs of 5-7 to produce synthetic diesel or other hydrocarbons from hydrogen and CO_2. Unlike methanol or ethanol, which are blended into the gasoline to reduce the CO_2 footprint of the respective fuels, the corresponding synthetic fuels are drop-in fuels which have almost the same chemical composition as fossil fuels (see Table 18) and could replace them completely. The company sunfire in German can be seen as leading in the area, see Box 3.

Box 3: Case Study Power-to-Liquids, sunfire, Dresden

The start-up sunfire is running the first power-to-liquid pilot plant worldwide in Dresden, Germany. With the combined operation of a steam-electrolysis reaching an electrical efficiency level of well over 90 % (for 10 kW_{el}) under pressure, a CO_2-Reverse Water Gas Shift-conversion and Fischer-Tropsch-synthesis, the plant can produce hydrocarbons from CO_2, water and renewable energy with an overall efficiency level up to 65 % (LHV H_2/kW_{el}). The hydrocarbons can serve the road traffic, shipping, aviation and chemical sector with fuels as gasoline, diesel, kerosene, methanol and methane.

Sunfire highlights especially the production of a synthetic diesel (“blue crude”) that already meets required characteristics and can be used without further adaptations for vehicles. The capacity of the plant for the synthetic diesel is 1 barrel per day. sunfire claims to save up to 3.14 tons of CO_2 for each ton of fuel produced by this approach.

The plant combines a Solid Oxide Fuel Cell (SOFC) and a SOE Cell. The so-called reversible Solid Oxide Cell (rSOC) operation is a SOFC and SOE cell in a single device. This combination makes it possible to supply electricity in time of renewable energy penury. Thus, the process can contribute to balancing power for the stabilization of the grid and can enable added value for the supply of electricity in decentralized regions. The first rSOC sold operates with a 100 kW SOEC power input and 50 kW SOFC power output.

Table 18: Characteristics of sunfire's synthetic diesel from pilot plant

Characteristics	Diesel (EN 590)	Sunfire blue crude
Gravimetric Density kg/m^3	820-840	780
LHV MJ/kg	42.5	44.7
Energy density [MJ/L]	34.9-35.7	34.9
Cetane number	>51	65-76
Further		Sulphur-free, aromatics content <1%

4.7.2.1 Energy demand per unit of synfuel production

Diesel and kerosene have the same energy density of 43.1 GJ/t. For the reaction scheme described above sunfire depicts 141 kJ energy demand for the water evaporation, 726 kJ for steam electrolysis and 41kJ for the reverse water gas shift. The exothermic Fischer Tropsch synthesis releases 147 kJ, which is sufficient to supply the water evaporation if efficient heat recuperation is ensured in the process configuration. Taking the 70% overall process efficiency, the energy demand is calculated as 66.3 GJ/t (or 18.4 MWh) in total, of which 62.8 GJ/t (or 17.4 MWh) are required for the electrolysis and 3.5 GJ/t for the RWGS.

4.7.2.2 CO_2 reduction per unit of synfuel production

A life cycle analysis of the sunfire process performed by University of Stuttgart[80] clearly shows the essential requirement of using low-carbon electricity for syndiesel production. The carbon footprint of syndiesel is close to 3 times that of fossil diesel, if the current German electricity mix is used. For 100% renewable electricity, emission reductions well-to wheel of 35% up to 85% have been quantified. Well-to-wheel emissions of conventional diesel amount to 88.6 g CO_2eq/MJ or 3.82 t CO_2eq/t diesel[78]. For kerosene, CO_2 emissions are at 71.5 g CO_2eq/MJ or 3.08 t CO_2eq/t[78]. Using a medium reduction potential of 60% compared to the fossil fuel, the CO_2 reduction is at 2.3 tCO_2eq per ton of syndiesel and 1.85 tCO_2eq per ton of synthetic kerosene. Table 19 provides an overview on the fuel demand and corresponding CO_2 emission reductions for different shares of synthetic fuels replacing diesel and kerosene.

Table 19: Impact of synthetic fuels

Synthetic fuels	2015	2020	2025	2030	2035	2040	2045	2050
Share synthetic fuels	0%	10%	25%	40%	50%	60%	75%	100%
Europe Diesel demand (IEA, 2DS) [PJ]	7463	7306	6441	5427	4688	4158	3536	3000
Syndiesel equiv. [mill. t]	173	170	149	126	109	96	82	70

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[80] http://www.lbp-gabi.de/files/sunfire_zusammenfassung.pdf

Syndiesel production [mill. t/year]	0	17	37	50	54	58	62	70
CO_2 emission reduction [mill. t/year]	0	39	86	115	125	133	141	160
Europe jet fuel demand (IEA, 2DS) [PJ]	2267	2187	1952	1704	1447	1359	1306	1290
Syn-jetfuel equiv. [mill. t]	53	51	45	40	34	32	30	30
Syn-jetfuel production [mill. t/year]	0	5	11	16	17	19	23	30
CO_2 emission reduction [mill. t/year]	0	9	21	29	31	35	42	55

4.7.2.3 Economics of synthetic fuel production

sunfire has calculated production costs for their synthetic diesel of 1.24 € per liter at electricity costs of 50€/MWh. A cost range of 1.2 to 1.5 €/L is therefore estimated for both fuels. This is to be compared to 25-60 €ct per liter for fossil crude exploration, showing a factor 2 higher production costs. Cost parity to fossil fuels is out of reach under the current framework conditions.

4.8 Methane from hydrogen and CO_2

To complete the options for hydrogen based processes, methanation has to be mentioned. This option is often referred to as Power-to-gas or Power-to-Methane. Synthetically produced methane or synthetic natural gas (SNG) is discussed as an energy storage option for intermittent power from renewable sources, as this storage option can use the existing gas storage and distribution infrastructure.

4.8.1 Low-carbon methane/SNG production from hydrogen and CO_2 (TRL 6-7)

Several large scale plants have been developed and installed in the 1970s as the oil crisis led to the assumption of running out of suitable fossil carbon feedstock[81]. Since then CO_2 (or CO) methanation did not attract intense attention. Lately however, a number of projects have been initiated and pilot plants have been built, in particular in Germany.[82] One example is Audi's E-Gas project, where wind power electricity is used for a PEM electrolyser and the formed hydrogen is converted with CO_2 separated from biogas to produce methane which is fed into the natural gas grid.[29] The methanation reactions from CO or CO_2 are as given below:

CO Methanation: $CO + 3 H_2 \rightarrow CH_4 + H_2O \qquad \Delta H^0 = -206$ kJ/mol
CO_2 Methanation: $CO_2 + 4 H_2 \rightarrow CH_4 + 2 H_2O \qquad \Delta H^0 = -165$ kJ/mol

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[81] Gert Müller-Syring et al., 2013, Entwicklung von modularen Konzepten zur Erzeugung, Speicherung und Einspeisung von Wasserstoff und synthetischem Methan in das Erdgasnetz
[82] http://www.powertogas.info/power-to-gas/pilotprojekte-im-ueberblick/?no_cache=1

Obviously large amounts of water are formed in this process, which subsequently need to be removed (e.g. by condensation) to obtain pure methane. The loss of hydrogen by water formation is an unavoidable drawback in the production of SNG as the amount of renewable hydrogen needed in the process doubles. The reaction itself is strongly exothermic and the produced heat can be used e.g. in SOE electrolysis.

The gas feed stream for methanation needs to be very pure and so the produced SNG will also only contain CO_2, H_2, H_2O and higher hydrocarbons as significant impurities. H_2O is removed by drying of the gas while CO_2 can remain in the SNG and the hydrocarbons can even be used to adapt the heating value of the product gas stream.

For easier storage and transport natural gas can be liquefied by cooling it to -162°C. Condensing the NG demands very clean natural gas, which means that prior to the cooling step the gas must be treated to remove other condensates, CO_2, water, and sulfur and mercury compounds[83]. As SNG contains significantly less of those impurities, liquefaction is easier and cheaper than for NG.

4.8.1.1 Electricity demand for of low-carbon SNG production

The production of methane from CO_2 via methanation requires 0.5 t hydrogen per t of methane. With an electrolysis efficiency of 4.3 kWh/Nm^3 H_2 the corresponding electricity demand per ton of SNG is calculated to be at 91.3 GJ or 25.4 MWh. The total energy demand is estimated to be 96.7 GJ (26.9 MWh), assuming an additional process energy demand of 5.4 GJ.

4.8.1.2 CO_2 reduction potential of low-carbon SNG production

The carbon footprint for fossil NG supply depends on many factors, such as source, world region, transport requirement etc. Fritsche et al.[84] quantify about 11 g CO_2eq/kWh NG for extraction and treatment of NG, for a NG heating value of 45 MJ/kg, this corresponds to 0.137 tCO_2eq/tNG. The carbon footprint of NG transport has to be added to this, depending on the transport distance.

To produce 1 t of methane, 0.5 t hydrogen and 2.7 t CO_2 are required. Electricity demand for electrolysis is at 91 GJ/t methane, causing the emission of 0.28 tCO_2/tmethane. The major impact originates from the capture and supply of CO_2 in this case, due to the high CO_2 demand. 1.15 tCO_2 have to be accounted. Including the footprint of other process steps estimated as 0.01 tCO_2/t methane and the footprint of CO_2 supply result in an overall CO_2 avoidance at 1.31 tCO_2/t methane.

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[83] Liquefied Natural Gas: Understanding the Basic Facts , US Department of Energy, 2005

[84] U. R. Fritsche, J. Herling, Energie- und Klimabilanz von Erdgas aus unkonventionellen Lagerstätten im Vergleich zu anderen Energiequellen, Darmstadt 2012.

4.8.1.2 Economics of low-carbon SNG production

The generation costs of SNG depend strongly on the price of electricity and on the operating hours of the methanation plants. Using only peak power, as is conceptually planned in many current PtG projects, the possible operation for methanation would be < 3000 h/year, imposing large economic hurdles. With PtG being currently imagined as "supplementary" technique for the storage of surplus power of renewable sources, operation hours down to 1200 hours per year are discussed. Several studies quantify the potential costs of production of methane via renewable electricity. The German Environmental Agency[85] calculated the costs for the production of CH_4 from renewable H_2 and CO_2 in 6 scenarios: operating hours of 1200 and 7000 h/year at electricity prices of 0, 50 and 90 €/MWh. Operating the methanation for 7000 h/year at electricity prices of 50 €/MWh resulted in production costs in a range of 2000 to 3500 € per ton of methane.

Reference fossil methane costs have been 154 € - 785 € in the OECD countries in 2014[86] Methanation will not be further considered in the scenario work of this study, as the main pathways previously described are based on syngas, without the need for methanation in a previous step. Direct synthesis of the targeted products from methane, such as methane to aromatics, without syngas and other intermediate steps is subject to intense fundamental research work, but methane activation has proven to be very challenging.

4.9 Comparison of the hydrogen based low-carbon synthesis routes

Table 20 provides an overview of the main results obtained for the low-carbon processes investigated in this chapter. Results are presented for the different target products, chemicals and synthetic fuels are separated. For the chemical products, the level of avoided CO_2 is very similar. Differences can be seen when avoided CO_2 is expressed as a function of required electricity or as a function of production costs. Avoided CO_2 per MWh is highest for urea followed by methanol and ammonia, which are on par. Ethylene, propylene and in particular the BTX yield lower efficiency in terms of CO_2 avoided per MWh. From the point of view of CO_2 avoidance costs, the merit order would be the same.

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[85] Umweltbundesamt, Treibhausgasneutrales Deutschland im Jahr 2050, July 2014; https://www.umweltbundesamt.de/sites/default/files/medien/378/publikationen/climate-change_07_2014_treibhausgasneutrales_deutschland_2050_0.pdf

[86] IEA, Key World Energy Statistics 2014

Table 20: Comparison of hydrogen based low-carbon synthesis routes

Product	Electricity [MWh]	CO_2 as feed [t]	Avoided CO_2 [t]	Costs [€]	Avoided CO_2 as kg	
Chemicals	per ton of product				per MWh	per €
Ammonia	12.5	-	1.71	700-800	137	2.1-2.4
Urea	8.1	0.73	2.05	450-500	253	4.1-4.5
Methanol	11.02	1.373	1.53	300-650	139	2.4-5.1
Olefins	26.6	3.2	1.89	670-1900	71	1-2.8
BTX	48.9	5.9	1.7	1300-2800	34	0.6-1.3-
Fuels	per ton of product			per L	per MWh	Per €
Diesel	18.4	3.15	2.3a)	1.2-1.5	125	1.3-1.6
Kerosene	18.4	2.85	1.85a)	1.2-1.5	100	1-1.2
SNG	26.9	2.7	1.31	2000-3500	49	0.4-0.7-

a) Well-to-wheel

Generally, the energy demand of these low-carbon synthesis routes is very high. In this sense, the low-carbon processes are not energy efficient as such, they just have a lower carbon footprint in the defined system. However, part of the high energy demand of the electricity-based low-carbon pathways can be attributed to the fact, that the target products are built-up from just water and CO_2, thereby not making profit of the high energy content of feedstock that is used in the alternative fossil processes. A comparison of the hydrogen-based low-carbon routes with the fossil reference route should therefore be performed on the basis of the total energy demand, i.e., in case of the fossil processes, including the energy content of the feedstock built-in the target product. This aspect and the low-carbon electricity of the hydrogen route are further discussed in chapter 10.

Another aspect of the depicted low-carbon routes is the potentially significant higher demand for noble metals and rare earth elements, that can be attributed to the provision of renewable electricity by e.g. wind power and the catalysts required for electrolyser cells. This impact has to be taking into account from a total resource efficiency point of view, but has not been investigated further in this study,

4.10 Availability of carbon dioxide as feedstock

The processes described in chapter 4 will depend on the availability of large amounts of CO_2 as feedstock, when deployed on a large scale. On the other hand, the power sector and the process industries strive for low-carbon technologies to to reduce CO_2 emissions to a large extend by 2050. This can potentially lead to a situation in the future, in which CO_2 availability from suitable point sources becomes a bottleneck. This will become more relevant with time, as low-carbon chemical production will increase and CO_2 emissions from industrial and power plant point sources will decrease. In order to investigate this potential limitation, projected supply has been compared with the demand as anticipated in the maximum scenario of this study. The maximum scenario developed in chapter 9.2, describes the upper limit of potential deployment, i.e. 100% of production based on low-carbon production, and therefore also defines the maximum demand for CO_2 as carbon source. Table 21 shows the CO_2 demand under the max scenario by 2050.

Table 21: Demand CO_2 as feedstock in the maximum scenario

CO_2 as feedstock [Mt]	2015	2020	2025	2030	2035	2040	2045	2050
Methanol as chemical	0	0.0	0.1	0.2	0.6	1.2	1.8	2.4
Urea	0	0.1	0.2	0.7	2.0	3.9	59	8.0
Ethylene/propylene	0	1.1	3.9	12.3	25.3	53.6	91.4	131.1
BTX	0	1.0	3.4	11.2	23.5	45.6	87.6	149.7
Total (chemicals)	**0**	**2.2**	**7.7**	**24.5**	**51.4**	**104.3**	**186.7**	**291.2**
Methanol as fuel	0	10.9	190	33.3	42.7	50.8	57.3	67.7
Syndiesel	0	26.7	47.1	79.4	102.9	136.9	181.1	219.5
Synkerosene	0	8.0	14.3	24.9	31.8	44.7	66.9	94.4
Total (fuels)	**0**	**45.6**	**80.4**	**137.6**	**177.3**	**232.4**	**305.3**	**381.6**
Total (chemicals + fuels)	**0.0**	**47.8**	**88.1**	**162.1**	**228.8**	**336.7**	**492.0**	**672.8**

In 2050, the CO_2 demand in this scenario will be at 291 Mt for chemical production and 381 Mt for the production of fuels, setting the upper limit to 673 Mt.

This is to be compared to the projected availability of CO_2 from large point sources. For this, the IEA ETP2015 2°C scenario has been considered, as this scenario already foresees strong CO_2 abatement efforts by all sectors. Table 22 shows the anticipated direct CO_2 emissions of large power plants and industrial point sources in Europe.

Table 22: CO_2 direct emissions from the European power sector and industrial sources in the IEA ETP2015 2°C model

CO_2 direct emissions	2015	2020	2025	2030	2035	2040	2045	2050
Industry	647	671	602	521	458	413	362	313
Power	1 315	962	700	430	199	103	76	69
Total	1 962	1 633	1 302	952	657	516	437	381

Evidently, the available amount of CO_2 would be sufficient to supply the demand of chemical production, even if 100% of the targeted petrochemicals would be produced by the described low-carbon technologies. In case of adding the production of synthetic transport fuels to chemical production, the CO_2 demand would surpass the available sources between 2040 and

2045. It has to be emphasized though, that this would only hold true for the scenario describing the maximum potential, which can be considered as unrealistic to achieve, given the high economic hurdles and the required high amounts of low-carbon electricity, which surpass the available power capacities. It should also be pointed out that the IEA scenario does not cover emissions from smaller industrial plants as well as from many small other sources such as biogas plants or breweries, which nevertheless can be suitable local sources for CO_2 supply.
The Ambitious scenario would only require 258 Mt CO_2 in 2050, including fuel production. It is therefore concluded, that carbon dioxide availability as feedstock is unlikely to become a bottleneck in the considered timeframe of the next 35 years. From a geographical point of view, local conditions might look different, as a match of production sites and sources needs to be achieved. In chapter 4.1.1.4 it was pointed out, that production plants based on electrolysis are likely to be smaller and decentralized, which potentially opens up many local or regional opportunities for new production sites. A detailed mapping of CO_2 sources, available sources of low-carbon power, chemical production facilities and other necessary infrastructure and utilities would be required for this. A mapping like this is beyond the scope of this study. Within the project “Value chains for CO_2 re-use”, in the Climate KIC programme ENCO$_2$re, a very useful map of CO_2 sources has been developed, which visualizes location, size and level of purity for CO_2 sources in Europe.[87]

Looking beyond 2050, i.e. a few more decades ahead, CO_2 from industrial sources might become a bottleneck. This would then require the implementation of direct air capture technologies.

5 Alternative synthesis pathways using CO_2

The previously described reaction pathways using CO_2 as carbon source are based on hydrogen as reaction partner. Other transformations of CO_2 utilise alternative reactants providing the necessary energy to enable CO_2 conversion. Of particular importance is the use of CO_2 as co-monomer for different polymers, as this opens the pathway to relatively large products with high added value. Figure 11 provides an overview of different CO_2-based products and the current status of deployment. The hydrogen based processes are included. Apart from urea, by far the largest current CO_2-based product other commercial processes include the synthesis of cyclic carbonates and salicylic acids, both produced in amounts below 0.1 million tons/year (TRL9).

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[87] http://enipedia.tudelft.nl/EPRTR/CO2_source_visualization.html

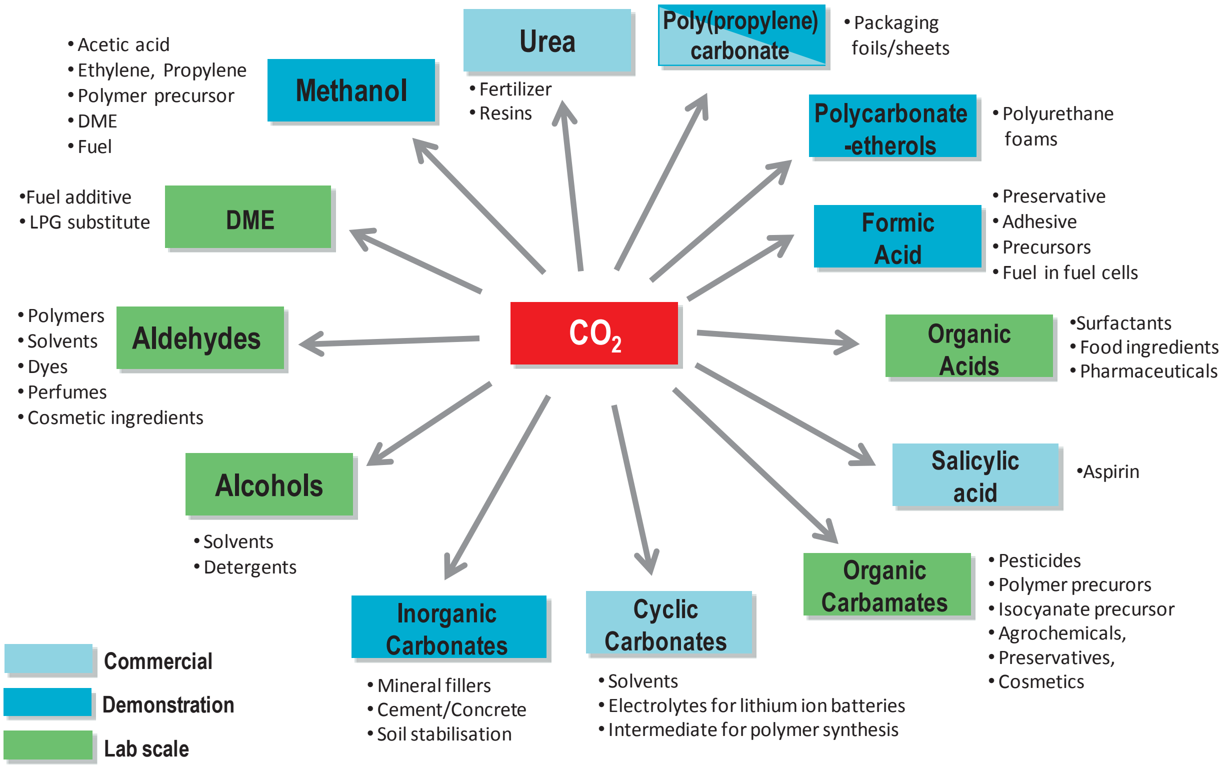

Figure 11: Target products of chemical CO_2 utilisation routes and status of deployment

Two groups of polymers can be produced using CO_2 as building block: poly(propylene)carbonate and polycarbonate etherols. Novomer Inc. in the US and Covestro (former Bayer MaterialScience) are active in this field with plants in operation (TRL7-9).

For formic acid a 1kg/day pilot plant for electrochemical CO_2 reduction has been erected by DNV, Norway and Mantra Energy Alternatives Inc. is building a 100 kg/day plant in Vancouver, British Columbia (TRL7). Mineral carbonation (mineralization) is used in semi-commercial plants for the treatment of industrial waste, contaminated soil, slags from metallurgy and production of cement-like construction materials (TRL7-9).

A large number of other processes is under investigation at lab scale, with substantially lower TRL. One approach to mention specifically because of a large potential is the direct synthesis of dimethylether (DME) from CO_2. The process should allow for a CO_2 reduction potential of 0.125 t CO_2 /t DME compared to the current state-of-the-art process with an intermediate methanol stage[88], corresponding to a 30% reduction. Further synthesis pathways investigated include the direct synthesis of sodium acrylate from ethylene and CO_2 or electrocatalytic processes to convert CO_2 to ethylene.

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[88] Final Conference "Technologies for Sustainability and Climate Protection – Chemical Processes and Use of CO_2", Berlin 2015, Book of Abstracts, p. 40, http://www.chemieundco2.de/_media/Book_of_Abstracts.pdf

6 Low-carbon chemical production based on biomass as feedstock

A completely alternative approach to avoid the use of fossil feedstock as carbon raw materials for the chemical industry is the use of renewable feedstock, i.e. biomass. Biomass is a valuable and limited resource and should be used in a sustainable way. A wide variety of sectors and areas compete for the use of biomass:

- Food and feed supply; obviously of the highest priority for sugar and starch containing biomass (1st generation biomass), as world population is increasing and demand for agricultural land use for food production will increase, making alternative use paths prohibitive.
- Energy; large amounts of biomass are used for the generation of electricity and heat by combustion of dry biomass incl. co-firing in power plants; furthermore, biogas plants and domestic heating contribute to this use path; lignocellulosic and waste biomass can be used in these applications, hence competition with food is low.
- Fuel; large amounts of renewable feedstocks are used for production of biofuels including bioethanol and FAME By 2020, the EU aims to have 10% of the transport fuels from renewable sources; the exclusive use of non-food biomass will be a future prerequisite.
- Material and carbon feedstock; this encompasses not only the industrial sector but also the wood (mainly for construction), and the paper industry.

A number of factors have to be considered for a sustainable use of biomass, This includes environmental aspects, such as soil erosion, water shortage, use of pesticides and eutrophication due to over use of fertilizers, land availability, indirect land use change, biodiversity etc. It is out of the scope of this study to investigate all these aspects in detail, but are considered with respect to future availability of biomass in chapter 6.7. For the large volume basic chemicals discussed in this study, a further consideration concerns the transport of biomass, which should be kept within certain limits to avoid high impact on carbon footprint, cost and logistics. Feedstock should be available within a certain radius of a production site, which is typically below 100 km.

The European chemical industry already uses renewable feedstock, in total about 8 Mt[89], corresponding to 10% of the total carbon feedstock requirement of 79 million tons. It is anticipated that biomass will play a larger role in the future, however limited by the availability of sustainable biomass and the strong use competition of different biomass use pathways.

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[89] Cefic 2013

6.1 Biomethanol production [TRL 6-7]

6.1.1 Biomethanol production process

Production of biomethanol follows the same pathway as coal-based methanol production, i.e. via gasification of the feedstock. A large variety of biomass feedstock can be used for this process and the net yield of wood-based methanol is 1.5 to 2 times higher compared to sugar and starch crops, based on the same heating value[90]

Figure 12 depicts a simplified process scheme. The biomass feed needs to be pre-treated. Depending on the biomass type, biomass contains up to 70% water, hence drying of biomass to 15% humidity prior to gasification is required. For gasification, different gasifier technologies are available, varying in gasification temperature and type of used biomass. Using a limited supply of oxygen during the feedstock heating improves the formation of syngas and reduces the amount of CO_2 and water. This can be an option to use oxygen from the electrolysis step of the processes described in chapter 4. Following the gasification, tars, dust and inorganic contaminants need to be removed in a gas cleaning step. Unprocessed light hydrocarbons can be further converted in a reformer. A water-gas shift is required to adjust the hydrogen to carbon monoxide ratio to the optimum for methanol synthesis.

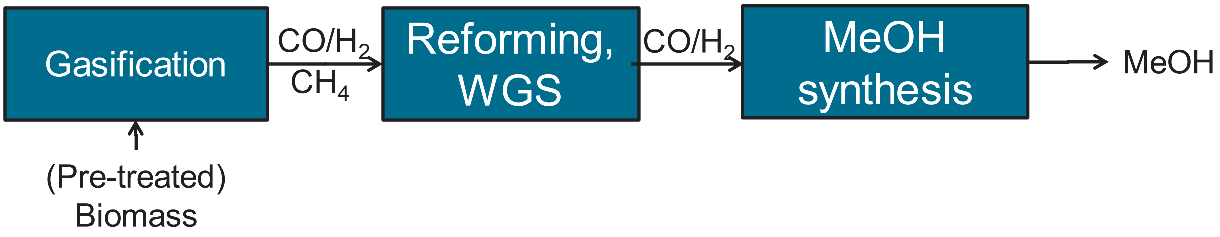

Figure 12: Process scheme of methanol production via biomass gasification

A first commercial scale biomethanol plant was announced in 2012 by VärmlandsMetanol AB in Hagfors, Sweden with ThyssenKrupp Engineering (former Uhde) as technology contractor.[91] The conceptual design and feasibility study based on a pressurised oxygen blown gasifier foresees 111 MW forest residue as feed to produce 100-110 kt fuel grade methanol, corresponding to a 66 -72% efficiency.

6.1.2 Energy and feedstock demand per unit of biomethanol production

Energy efficiency of the methanol from biomass process is lower compared to the incumbent natural gas process, due to the higher effort in biomass pre-conditioning, the lower hydrogen to

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[90] H.-J. Wernicke, L. Plass, W. Reschetilowski, Raw materials for methanol production, in: M. Bertau, H. Offermanns, L. Plass, F. Schmidt, H.-J. Wernicke (Eds.), Methanol: The Basic Chemical and Energy Feedstock in the Future.

[91] http://www.varmlandsmetanol.se/dokument/History%20March%2012.pdf

carbon ratio of the feedstock and the higher ash and char contents. Process efficiency of the biomass based process is between 50-60%.[92] Azar et al. estimated a conversion efficiency of woody biomass to methanol of 60%.[93] The above mentioned VärmlandsMetanol plant claims a 66%-72% efficiency, which would be on par with the NG to methanol efficiency at 64%-72%[92], but this value probably does not include feed preparation steps. As conservative estimate, a 60% efficiency has been assumed. The energy demand of the biomass route can then be calculated as 14.6 GJ/ t methanol compared to 12.5 GJ/t methanol from NG. For this efficiency, an amount of 2.6 tons dry wood biomass would be required as feedstock per ton of methanol[94].

6.1.3 CO_2 reduction per unit of biomethanol production

Estimates of CO_2 emissions from biomethanol production vary widely in the literature, depending on different assumptions. A German study[95] estimated 0.64 tCO_2eq/t methanol for a production based on short rotation coppice, and 0.56 tCO_2eq/t for forest residues as feedstock, compared to methanol from natural gas at 0.84 tCO_2eq/t methanol. Taking the higher emission value as a conservative assumption this corresponds to 0.2 t CO_2eq/t methanol or 24% emission reduction. In addition, the biogenic carbon sequestered in methanol corresponds to 1.37 tCO_2, yielding an avoidance potential of 1.57 tCO_2/tmethanol.

Box 4: Carbon footprint of biomass feedstock

Analogous to the fossil and hydrogen-based processes discussed in the previous chapters, the CO_2 emissions of biomass-based processes need to be based on a cradle-to-gate analysis, i.e. have to include the feedstock production. In the case of agricultural or forestry biomass, this includes cultivation, harvesting and transport, in case of residual/waste biomass, the lifecycle starts at the factory gate of the supplying source. Life cycle assessment of biomass tends to be complicated, as many local and seasonal factors determine the result. In addition to the carbon footprint, many other factors such as land use change, biodiversity, water shortage etc. have to be considered. In this study, LCA data from different studies and the well-to-tank report of the EU Joint Research Center (reference 78) have been used. Caution is recommended in trying to generalize these LCA results.

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[92] L. Bromberg and W.K. Cheng, Methanol as an alternative transportation fuel in the US:Options for sustainable and/or energy-secure transportation; retrieved October 2016, http://www.afdc.energy.gov/pdfs/mit_methanol_white_paper.pdf

[93] C. Azar, K. Lindgren and B. A. Andersson, Global energy scenarios meeting stringent CO_2 constraints—cost-effective fuel choices in the transportation sector; Energy Policy, 2003, 31, 961-976.

[94] based on 18.5 MJ/kg wood at 30% moisture content, from reference 78.

[95] S. Majer, A. Gröngröft, 2010, Environmental and economic assessment of for biodiesel production, Deutsches BiomasseForschungsZentrum, Leipzig, Germany, DBFZ project number 3514000.

Carbon from biomass sequestered in the target product is generally counted as negative emissions in the production phase of a biomass-based product. These negative CO_2 emissions correspond to the positive emissions on total combustion of the target product at the product's end of life. The latter is included in the well-to-wheel data, used for comparing different fuels.

6.1.4 Economics of biomethanol production

For basic chemicals, the raw material costs usually represent 60–70% of the production costs. Hence production cost of biomass-derived methanol is largely dominated by the relatively high costs of agricultural and forestry biomass in comparison to fossil feedstocks.

The costs of methanol production from biomass has been quantified in many studies and ranges from 160€/t methanol[96] up to 940€/t[97], very much depending on plant setups and local conditions. Cost estimates at a higher annual production capacity are on the lower end, indicating economy of scale effects. Production costs for biomethanol from waste streams are slightly lower compared to wood, i.e. between €200-500 per ton.

Compared to cheapest fossil fuel based production, biomethanol production costs are at least 1.5 times higher, capital cost per unit of capacity is at least 3.4 times higher than the capital cost of natural gas based plants.[98] It was also estimated that biomethanol plants are about 1.8 times more expensive than bio-ethanol facilities on the basis of the same energy output.[92]

6.2 Bioethanol production [TRL7-9]

While ethanol is not among the petrochemical products targeted in this study as such, the production of bioethanol actually comprises one of the major renewable feedstock pathways in Europe. Furthermore, bio-ethanol would be the feedstock for a subsequent synthesis of bio-ethylene and is a major biofuel contributing to the low-carbon transportation fuel production addressed in this study.

The EU is the world's third largest producer of ethanol after Brazil and the US, at 6.4 billion litres in 2015.[99]. Ethanol production in Europe has shown strong growth rates in recent years, however, a decline has occurred from 2014 (6.9 billion litres) to 2015. The same annual growth rate of 1% as for the petrochemicals has therefore been used for the scenario work.

First generation bioethanol is produced from crops such as wheat, corn, sugar cane and sugar beet. In Europe, 37% of the ethanol produced was from corn (maize), followed by wheat (33%) and sugar beets (20%)[99]. Due to the food competition, 1st generation biofuels are more and

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[96] C. N., Hamelinck, A. P. C. Faaij, Production of methanol from biomass, Utrecht University 2006, NWS-E-2006-387.

[97] L. Tock, M. Gassner, F. Maréchal, Thermochemical production of liquid fuels from biomass: Thermo-economic modeling, process design and process integration analysis, Biomass and Bioenergy 2010, 34, 1838-1854.

[98] IEA-ETSAP and IRENA Technology Brief I08, Production of Biomethanol, January 2013.

[99] ePure, http://epure.org/media/1466/epure-key-figures-2015.pdf

more perceived critically and the European Commission has proposed to limit 1st generation biofuel produced at 7% of energy use in transport. Bioethanol production is at TRL9 for sugar and starch containing crops, but is considered at TRL7 for lignocellulosic biomass (2nd generation biofuels).

6.2.2 Bioethanol production process

Production of ethanol is basically based on the fermentation of sugar-rich biomass, followed by distillation. The process scheme is depicted in Figure 13.

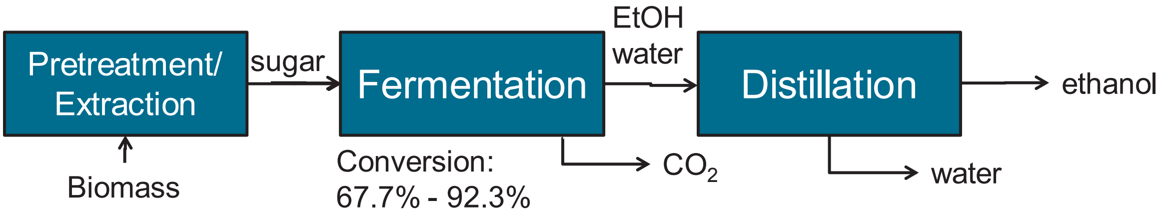

Figure 13: Process scheme of bioethanol production

The process starts with biomass pre-treatment, i.e. extraction of sugar. For sugar beet, the most used sugar crop, sugar is extracted via heat extraction and vaporisation. Starch, from the starch crops wheat, maize or other cereals needs to be hydrolized into monosaccharides (saccharification). The starch crops are crushed and mashed, then enzymes (e.g. amylases) are added to the mash which dissolve the starch into sugar. Lignocellulose (agricultural and wood residues, wood from forestry, short rotation coppices and lignocellulosic energy crops, such as energy grasses and reeds) require a more complex pre-treatment, due to the different components, i.e. cellulose, hemicellulose and lignin. As common pretreatment method, steam explosion is applied, which breaks the structure of the lignocellulosic material through an hydrothermal treatment, using high pressure steam at high temperature for a short time followed by rapid decompression. Alternative methods use supercritical carbon dioxide. The cellulose and the hemi-cellulose are separated from the lignin, and saccharification is induced through enzymatic hydrolysis with cellulases and hemi cellulases. The C6 sugars can be fermented by common yeasts while C5 sugars need specific microorganisms to get fermented. Lignin is currently usually separated and dried to be used as a fuel for the process or for power generation.
The reaction from glucose is as follows:

$$C_6H_{12}O_6 \dashrightarrow 2\ C_2H_5OH + 2\ CO_2$$

The fermentation yields a diluted aqueous ethanol solution with about 12% ethanol content. At this point the fermentation stops due to the toxic effect of ethanol on the yeasts. Ethanol at 96% is obtained by distillation. To be used as biofuel, 98.7%m/m are required. For this, the remaining azeotropic water is removed by dehydration.

6.2.3 Energy and feedstock demand per unit of bioethanol production

For the energy demand, a detailed study has been provided for different biomass feedstocks in the well-to-wheel report of the JRC[78], including cultivation, feedstock preparation and ethanol production. For sugar beets as feedstock, the energy consumption depends on the process configuration, i.e. the utilisation of the pulp leftover after filtration of the diluted ethanol liquor and the distillation residues ("slops") for electricity co-generation and biogas production respectively. If credits for these contributions are included, energy consumption well-to-tank is at 0,89 MJ per MJ ethanol or 23.85 GJ/t ethanol respectively, if not, it amounts to 1.42 MJ/MJ ethanol or 38 GJ/t ethanol. For lignocellulosic biomass wood has been used, based on short-rotation forestry of poplar or willow on agricultural land. In this case, 1.78 MJ per MJ ethanol or 47.7 GJ/t ethanol are required. For comparison, the fossil ethanol production via ethylene production from Naphtha and dehydrogenation to ethanol results in 21.9 GJ/t ethanol.[78]

Stoichiometrically, 51.1% of glucose is converted to bioethanol, meaning that a minimum of 2.12 tons of glucose are needed to produce 1 ton of ethanol. Glucose fermentation is a well-known process and can produce ethanol at 92.3% yield, resulting in an overall biomass utilisation efficiency of 47.2%.[100] Using wheat straw as feedstock, 0.29 g ethanol per g straw have been shown at a conversion rate of 86%[101] indicating a biomass utilisation efficiency of 29% for lignocellulosic material as feedstock, i.e. 6.75 tons of wheat straw equal 1 ton of ethanol. For wood, 6.05 tons are required.

Bioethanol production today is exclusively based on sucrose and starchy biomass. For the scenarios in this study, it has been anticipated that the raw materials for future production of bioethanol will change to lignocellulosic biomass, and that the share of lignocellulosic biomass will continuously increase to 25% in 2050.

6.2.4 CO_2 reduction per unit of bioethanol production

CO_2 emissions well to tank have also been taken from reference 78. Emissions are between 16.2 and 38.6 $kgCO_2eq$/GJ ethanol (0.43 and 1.03 tCO_2eq/t ethanol) for sugar beet, depending on the process configuration, i.e. if utilisation of the pulp and distillation residues ("slops") for electricity co-generation and biogas production respectively is taken into account. In the case of wood, emissions are at 21.2 $kgCO_2eq$/GJ ethanol or 0.57 tCO_2eq/t ethanol. The footprint of the fossil route is at 1.06 tCO_2eq/t ethanol, roughly double of the CO_2 footprint of the most

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[100] nova paper #8 on bio-based economy 2015-11; Definition, Calculation and Comparison of the "Biomass Utilization Efficiency (BUE)" of Various Bio-based Chemicals, Polymers and Fuels

[101] B. C. Saha, N.N. Nichols, N. Qureshi, G. J. Kennedy, L. B. Iten, M. A. Cotta, Pilot scale conversion of wheat straw to ethanol via simultaneous saccharification and fermentation, Bioresource Technology. 2014, 175:17-22.

efficient biomass routes. Biogenic carbon sequestered in bioethanol corresponds to 1.91 tCO_2/t ethanol.

As ethanol is included as a fuel in subsequent scenarios, the carbon footprint of bioethanol production has also to be compared to the production footprint of gasoline. The latter is at 12.6 $kgCO_2eq$/GJ produced gasoline[78], which is **41 % lower** than the footprint of bioethanol production. However, this is largely overcompensated by the high gasoline emissions during fuel use.

6.2.5 CO_2 reduction for (partially) replacing gasoline by bioethanol

The European EN228 specification for gasoline allows blending of ethanol up to 10%. Where high ethanol blends (e.g. E85) are used, they can only be used in vehicles specially adapted to use such fuels. For gasoline, CO_2 emissions well to wheel amount to 87.1 g CO_2/MJ. For ethanol in the beet route scenario depicted above, emissions well to wheel amount to 17.8 g CO_2/MJ.[78] In total, this corresponds to a reduction of 69.3 g CO_2/MJ of fuel.

6.2.6 Economics of bioethanol production

Production costs of ethanol are largely determined by the biomass feedstock prices, which can account for 55 - 80% of the final price of ethanol. SenterNovem estimated production costs for large plants in Europe at 0.50-0.55 €/L for sugar beet based processes, 0.55-0.60 €/l for grain based processes, and 0.45-0.55 €/L for processes using residual starch streams.[102] Projections towards 2020 are estimated at 0.45-0.50 €/L for sugar beet based processes, 0.50-0.55 €/L for grain based processes and 0.40-0.50 €/L for processes using residual starch streams.

The International Renewable Energy Agency (IRENA) estimates bio-ethanol production from lignocellulosic biomass to cost about 750 US$/t or 975 €/t (2012), which would correspond to 0.77 €/L.[103]

6.3 Bioethylene production [TRL8-9]

6.3.1 Bioethylene production process

Bioethylene production is based on bioethanol as feedstock and hence follows the process steps discussed in the previous chapter. The general process scheme is depicted in Figure 14.

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[102] Biofuels in Europe,SenterNovem 2006

[103] IEA-ETSAP and IRENA Technology Brief I13, Production of Bio-ethylene, January 2013

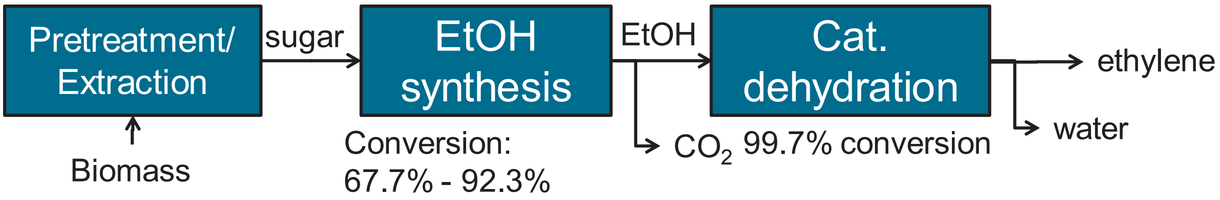

Figure 14: Process scheme for bioethylene production

Using bioethanol as feedstock, bioethylene is produced via dehydration of the ethanol over an alumina or silica-alumina catalyst at 300°C in a fixed bed or in a fluidized bed reactor. As workup, a gas separation is required to remove gaseous by-products and an alkaline scrubbing to remove oxygenates. One ton of bio-ethylene requires 1.74 t of (hydrated) ethanol[104]. Conversion yields are at 99% with 97% selectivity to ethylene. The reaction is endothermic and requires a minimum theoretical energy of 1.68 gigajoules (GJ) per ton of bioethylene.[104]

The current largest bioethylene producer is Brazil, but the concept is also implemented in Europe. In 2014, Axens, Total and IFP Energies Nouvelles announced an technology for bioethylene production through dehydration of bioethanol under the technology brand name Atol™, to produce of polymer grade bio-ethylene.[105] The processes can omit the alkaline workup due to the specially developed catalyst showing very high ethylene selectivity.[106]

As alternative concept the gasification of biomass to syngas, followed by methanol production and MTO has to be mentioned (see chapter 6.1), but this process is not favourable in terms of CO_2 emissions (compare chapter 6.4.4).

6.3.2 Energy and feedstock demand per unit of bioethylene production

For the entire process chain including production of 1.74 t ethanol followed by the ethylene production an energy demand of 85.5 GJ/t ethylene results, which is very high compared to 21.9 GJ/t ethylene from oil via naphtha (incl. primary feedstock production).[6]
It is assumed that ethylene production would be based on wood. Feedstock demand in this case is at 10.5 t/t ethylene.

6.3.3 CO_2 reduction per unit of bioethylene production

The fossil ethylene production route causes 1.15 tCO_2eq/t ethylene including feedstock production.[6] For bioethylene production, the carbon footprint of the bioethanol feedstock production (including biomass raw material production) and the emissions caused by the

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[104] N. K. Kochar, R Merims, A. S. Padia, Gasohol Developments: Ethylene from Ethanol. Chemical Engineering Progress 1981, 77 (6), 66-71.
[105] http://news.bio-based.eu/total-confirms-will-produce-bio-ethylene-bio-ethanol/
[106] The launch or a new bioethylene production process, Chem. Eng. 2014, May, 11.

ethanol dehydration process have to be taken into account. In terms of raw material and bioethanol production, the 0.57 tCO_2eq/t ethanol for wood from chapter 6.2.4 have been used. As 1.74 t ethanol per t ethylene are required, the bioethanol production step prior to ethylene synthesis causes around 1 tCO_2eq/t ethylene. It is estimated that at least 0.2 tCO_2eq/t is emitted in the ethylene production process, which makes the process related CO_2 emissions relatively close to the fossil process. For wood or waste biomass reduced emissions of the biomass route can be anticipated. The biogenic carbon sequestered into the product, which is counted as negative emission stoichiometrically amounts to 3.14 tCO_2/t ethylene. The amount of avoided CO_2 compared to the fossil process is hence at 1.95 tCO_2/t ethylene.

A case by case analysis of the carbon footprint is strongly advised for bioethylene production, as the carbon footprint depends on the type of biomass used and the local production logistics and infrastructure.

6.3.4 Economics of bioethylene production

The International Renewable Energy Agency quantifies the production costs of bioethylene in the EU at 3250 €[107]. The biomass feedstock accounts for about 60% of the bio-ethanol production costs. The bio-ethanol costs in turn account for about 60-75% of the bio-ethylene production costs.[103] Bio-ethanol production from lignocellulosic biomass was estimated to cost about 975 €/t ethanol, assuming mature technical and economic conditions. This leads to a bio-ethylene production cost of 2.250 to 2.800 €/t ethylene which would be in the range of the current thermochemical production route at about 2,500 €/t.

6.4 Biopropylene production [TRL 6-7]

6.4.2 Biopropylene production processes

Biopropylene production can be considered as a further step following bioethylene production.

In Brazil, Braskem has announced a production plant for bio-based polypropylene at 30 000 t/a scale.[108] The two-stage process is based on dimerization of ethylene to 1-butene, isomerization to 2-butene, and metathesis with ethylene. A new catalyst was reported to allow realization of the process even in one stage.[109]

As for ethylene, the route via biomass gasification, methanol synthesis and MTO/MTP is also available (see chapter 6.1).

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[107] Based on ref.. 103; the report provides numbers in US$; exchange rate of 1.30 €/US$ (2012) has been used.

[108] http://www.icis.com/blogs/green-chemicals/2010/11/braskem-to-build-bio-pp-plant/

[109] N. Popoff, E. Mazoyer, J. Pelletier, R. M. Gauvin, M. Taoufik, Chem. Soc. Rev. 2013, 42, 9035–9054; DOI: 10.1039/c3cs60115c

Other routes are available at lower TRL, e.g. the fermentative production of propanol or isopropanol, followed by dehydration[110], the direct fermentative production of propylene, as investigated by Global Bioenergies[111] or the catalytic conversion of (bio)ethanol to propylene at Sc-loaded In_2O_3[112].

6.4.3 Energy and feedstock demand per unit of biopropylene production

The synthesis route via gasification to methanol requires 2.6 t dry biomass/t methanol and the MTO route stoichiometrically requires 2.28 t methanol/t propylene. Total biomass demand is therefore at least 5.9 t per t propylene. Energy demand of the different process steps is additive, and amounts to 95.5 GJ/t propylene of which 90.5 GJ are allocated to the synthesis of the required methanol feed and 5 GJ/t HVC for the MTO process.

The second route, dimerization/isomerization with subsequent metathesis, the energy demand is estimated based on the stoichiometric bioethylene demand, as no further information on the process specific energy requirement and related emissions is available. The corresponding energy demand would be 130 GJ/t propylene. This can be considered as a good approximation, as the energy consumption will be driven by the ethylene synthesis sequence.

6.4.4 CO_2 reduction per unit of biopropylene production

As for the process energy, the carbon footprint is composed of the emissions of the different process steps. As a result, process related CO_2 emissions are at 1.86 tCO_2eq/t propylene, which is a factor 2.5 that of the fossil route via naphtha steam cracking. Sequestered bio-based carbon amounts to 2.09 tCO_2eq/t propylene, which slightly overcompensates the process emissions, however, the gain is low. This route is therefore considered as relatively unfavourable in terms of energy and resource efficiency, given the high biomass demand.

For the dimerization/isomerization with subsequent metathesis process related emissions of 1.65 t CO_2/t propylene would result, which is also well above the fossil route at 0.76 t.

6.5 BTX production from biomass [TRL6-7]

6.5.1 BTX production process

The production of BTX from biomass can follow several routes. As the most developed route, gasification of biomass, methanol synthesis and methanol to aromatics is used. Figure 15 shows the process sequence.

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[110] A. J. J. Straathof, Chem. Rev. 2014, 114, 1871–1908. DOI: 10.1021/cr400309c

[111] J. Lane, Biofuels Digest, March 6, 2014.

[112] M. Iwamoto, S. Mizuno, M. Tanaka, Chem. Eur. J. 2013, 19, 7214–7220.

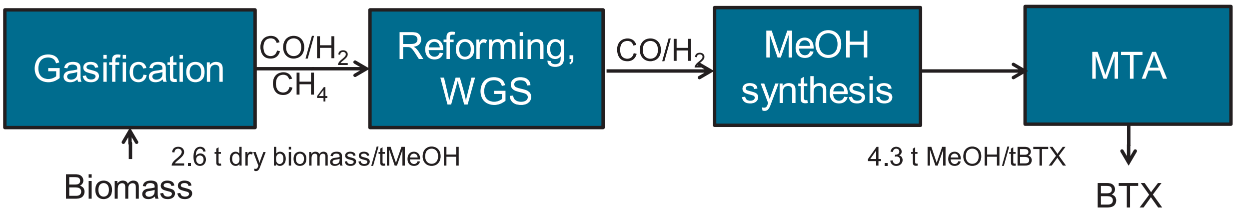

Figure 15: Process scheme for BTX production from biomass via gasification

The individual process steps have already been described in chapters 6.1 (biomass to methanol) and 4.6.2 (methanol to aromatics).

An alternative synthesis of p-xylene (pX) can be performed in 4 steps from bioethanol derived ethylene, followed by Ir-catalyzed trimerisation to 1-Hexen, dehydrogenation to Hex-2,4-diene followed by Diels-Alder-addition with another ethylene molecule and finally Pt-catalyzed dehydrogenation. A yield up to 65% has been reported[113] In total 5 ethylene molecules are required to synthesize one molecule of pX.

A seemingly obvious pathway is only available at very low TRL: the selective degradation of lignin thereby releasing the contained aromatic structures. All attempts based on pyrolysis or hydrogenation have so far failed to result in a technically viable process. All proposed process routes are extremely unselective and yield a large product spectrum.[114]

As another option, fast pyrolysis of lignocellulosic biomass has been investigated and significant yields of aromatic compounds have been reported. The mixture contains different aromatics with toluene, benzene, and xylenes as major components.[115] Anellotech and KiOR are attempting to implement this approach, but KIOR stated to be unable to achieve commercial-scale production. Anellotech's process, developed in collaboration with Johnson Matthey and IFP Energies Nouvelles is based on the research results of G. W. Huber, University of Wisconsin, Madison, who has reported aromatics yields from wood of up to 20% (C-content).

6.5.2 Energy and feedstock demand per unit of BTX production from biomass

Both synthesis routes have been assessed in terms of energy demand and CO_2 emissions. As depicted in Figure 15, the synthesis route via gasification to methanol requires 2.6 t dry biomass/t methanol and the MTA route requires 4.3 t methanol/t BTX. Total biomass demand is therefore at least 11.2 t per t BTX. Energy demand of the different process steps is additive, and amounts to 72 GJ/tBTX of which 67 GJ are allocated to the synthesis of the required

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[113] T. W. Lyons et al., J. Am. Chem. Soc. 2012, 134, 15708 – 15711, DOI: 10.1021/ja307612b

[114] K. Wagemann, Production of Basic Chemicals on the Basis of Renewable Resources as an Alternative to Petrochemistry?

[115] T. R. Carlson, Y.-T. Cheng, J. Jae, G. W. Huber, Energy Environ. Sci. 2011, 4, 145.

methanol feed and 5 GJ/ for the MTA process. For the Diels Alder process, 2 t ethylene/t pX are required, yielding an extremely high energy demand of the bimomass-based process chain of 174 GJ/t. This is to be compared with the SEC of fossil BTX production, which is around 7 GJ/tHVC (see chapter 4.6.1).

6.5.3 CO_2 emissions per unit of BTX production from biomass

As for the process energy, the carbon footprint is composed of the emissions of the different process steps. As a result, process related CO_2 emissions are at 2,21 tCO_2eq/tBTX for the Diels-Alder route and 2.6 tCO_2eq/tBTX for the MTA route, which is factor 2 to 3 of the fossil route at 0.84 tCO_2eq/tBTX. Overall emission reductions would therefore originate only from the bio-based carbon sequestered in the products, which amounts to 3.3 tCO_2eq/tBTX, resulting in a total carbon footprint of -0.7 tCO_2eq/tBTX for the MTA route or -1.54 tCO_2eq/tBTX avoided CO_2 compared to the fossil route.

Due to very high energy and feedstock demand, BTX production from biomass based on the two investigated routes is not considered to be beneficial from an energy/resource efficiency point of view. The alternative production routes briefly described above, selective lignin decomposition and fast pyrolysis, need to be investigated further. This can be regarded as a high priority for a low-carbon chemical production strategy, in particular, as the hydrogen based route described in chapter 4.6.2 is also extremely energy demanding.

6.6 Comparison of the biomass-based synthesis routes

Different routes using renewable feedstocks to produce large volume chemicals have been investigated in this chapter. Table 23 provides a summary of the main results obtained.

Table 23: Comparison of biomass-based synthesis routes

Product	Energy demand [GJ]	Biomass as feed [t]$^{a)}$	Δprocess related CO_2 emissions [t]$^{b)}$	Biogenic carbon sequestered as CO_2 [t]	Costs [€]	Avoided CO_2 [kg]	
Chemicals		per ton of product				per t biomass	per €
Methanol	14.6	2.6	-0.2	-1.37	200-500	600	3.1-7.8
Ethylene	85.5	10.5	+0.05	-3.1	2250-2800	290	1.1-1.3
Propylene	95.5	5.9	+1.1	-2.09	2200-2500	170	0.4-0.45
BTX	72	11.2	+1.76	-3.3	>3000	139	<0.46

Fuels		per ton of product			per t	per €
Bioethanol	47.7	6.1	Well-to-wheel emissions: 1.86	975	305	1.9

a) Dry wood has been used as reference

b) compared to the fossil reference process

Results are presented for the different target products. Bioethanol has been included as fuel. From a biomass use and economic point of view, Biomethanol and bioethanol represent the most meaningful use paths of biomass among the investigated routes. The olefins and in particular BTX synthesis based on the suggested multi-step synthesis pathways are characterized by very high biomass demands per ton of product and costs of CO_2 avoidance. In particular the BTX synthesis from biomass shows substantially higher process related emissions than the fossil based processes.

The main reason is the mentioned large demand of feedstock for these processes, which is utilised in a relatively inefficient way. A paper by Nova describes the “biomass utilisation efficiency” (BUE) as a means of describing the percentage of initial biomass ending up in the end product based on the molar mass of the reactant and target bio-based product.[100] The authors for instance conclude a low BUE of 28.6% for polyethylene, due to the fact that the ethylene molecule contains no oxygen. Biomass or finally sugar use in such a case encompasses the removal of all oxygen as CO_2 from the sugar structure, thereby also eliminating a large number of carbon. This is actually the case for all large petrochemicals included in this study. The BUE also tends to decrease with the number of synthesis steps, and the biomass based routes described in this study usually encompass several steps. It can be concluded, that the production of drop-in petrochemicals from biomass is a rather inefficient way of using biomass, with a BUE being generally low. This fact is even more relevant taking into account the limited availability and competition of use pathways of sustainably produced non-food biomass or waste biomass. This is discussed in chapter 6.7.

Much higher efficiencies can be achieved for dedicated biomass-based synthesis routes that maintain the functional units of the feedstock molecules, e.g. oxygen-rich and carbonated molecules such as polylactic acid and succinic acid. In light of the limited availability of biomass as a valuable raw material it is therefore strongly recommended to strengthen the deployment of such routes. The situation might be assessed differently for complex biorefineries, in which different feedstock and production streams are coupled in an intelligent manner.

6.7 Available biomass feedstocks

As basis for the scenario work described in chapter 9, it is important to estimate the future availability of biomass, in order to define reasonable ambitions in terms of the implementation of biomass-based production routes. A number of studies have investigated the availability of biomass. As a comprehensive overview, the “Atlas of EU biomass” developed in the EU Biomass Futures project has been taken as basis[116]. The report identifies different biomass feedstock and provides an inventory of data to quantify and map the technically constrained biomass potentials. For the estimate of potentials, the report takes different sustainability criteria into account that will constrain the future availability of biomass. Two scenarios, “reference” and “sustainable” are provided, the sustainability scenario considering stricter sustainability criteria, e.g. GHG mitigation requirement including compensation for emissions from indirect land use changes caused by biomass cropping in the EU. While the report focuses on bioenergy, it is considered as relevant also for the purpose of this study. An overview of the projected biomass availability according to different biomass classes is provided in Table 24.

Biomass potentials are expected to increase, in particular in the reference scenario but will consolidate between 2020 and 2030. In the sustainability scenario the potential will even decline because of constraints on access to land. It is important to note, that the contribution of the waste sector is expected to decline

Within the scope of this study, it is expected, that this trend will continue and no additional potentials can be expected beyond 2030, as regulatory constraints will likely increase and pressure from food competition will increase. A biomass potential in Europe of 350 to 400 Mtoe is therefore expected. This is also in agreement with a metastudy by Zeddies et al.[117], which compares biomass potentials from different studies. A biomass availability in Europe of 15 EJ is projected in 2050, corresponding to 358 Mtoe.

The available biomass will of course have to be distributed to a variety of competing use options, as described in the introduction of chapter 6. For the scenario work, the availability of biomass is considered and the relative share of biomass use as function of the ambitions is described.

24: Biomass availability in Europe, adopted from Ref. 116.

EU 27; Mtoe	Basis 2005	reference 2020	sustainable 2020	reference 2030	sustainable 2030
Wastes	42	36	36	33	33
Agricultural residues	89	106	106	106	106

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[116] Biomass Futures, Atlas of EU biomass potentials, 2012

[117] J. Zeddies, N. Schönleber, Literaturstudie „Biomasse - Flächen- und Energiepotenziale“, December 2014

Rotational crops	9	17	0	20	0
Perennial crops	0	58	52	49	37
Landscape care wood	9	15	11	12	11
Roundwood	57	56	56	56	56
Additional harvestable roundwood	41	38	35	39	36
Prim. forestry residues	20	41	19	42	19
Sec. forestry residues	14	15	15	17	17
Tert. forestry residues	32	45	45	38	38
Total	**314**	**429**	**375**	**411**	**353**

7 Valorization of gaseous emissions and side streams of other sectors (Industrial symbiosis)

The term industrial symbiosis refers to collaborations between different sectors or enterprises, in which materials, energy, water and byproducts/waste are exchanged. Typically, side streams of one company or sector is used as raw material or energy supply by another sector or company.

One element of industrial symbiosis highlighted in chapter 3.1 is the electricity-based heating and steam generation by the chemical industry as demand side management and service to the power sector. The fast response time of this technology allows valorization of intermittent surplus supply of renewable electricity, hence improving flexibility in the power supply. In return, the chemical industry can benefit from periods with low electricity prices.

Another element already mentioned previously is the valorization of off-gases provided by other industries for chemical production. The technologies described in chapter 4 are characterised by a high demand for hydrogen as well as carbon dioxide as feedstock. As many processes involve syngas, sources of carbon monoxide are also important to consider.

This chapter therefore aims at describing industrial symbiosis with other process industries, in which the chemical industry valorises side process gas streams of H_2, CO and CO_2 emissions from these other sectors.

7.1 Sources of CO_2

A number of industrial sources of CO_2 are to be considered for CO_2 conversion in low-carbon chemical production. Table 25 provides an overview of large industrial CO_2 sources with typical amounts and CO_2 concentrations. From a carbon capture point of view, sources of high concentration appear most attractive, as energy demand but also cost of capture depend on the concentration of CO_2.

Table 25: Large industrial CO_2 sources and key parameters

Table 25: Large industrial CO_2 sources and key parameters

CO_2 source	Total available amount in EU [Mt] [118]	Amount per unit production	Typical CO_2 concentrations in source gas [vol. %]
Power plants	1225	0.7-0.8 t CO_2/MWh	3-4; 12-14 for IGCC
Steel plants	110	1.2-1.5 t CO_2/t steel	14-27
Cement plants	114	0.6-1.0 t CO_2/t cement	15-33
Chemical plants	example NH_3 23	1.8 t CO_2/t NH_3	close to 100

Many current chemical processes, especially those via syngas production are emitting substantial amounts of CO_2 due to the nature of the respective process and its feedstock. Some of these production routes provide relatively pure CO_2, and such sources should be valorized as first priority. Processes providing close to 100% CO_2 include ethylene oxide, ammonia production (the latter often directly utilising the CO_2 for subsequent urea production), natural gas cleaning, but also fermentation processes, e.g. bioethanol production. Other industrial sources include steel and cement plants, providing off gas concentrations of CO_2 considerably lower, but often still higher than those in flue gas from fossil fired power plants.

Depending on the target product of the low-carbon chemical process, hydrogen and CO_2 supply require a specific match of the feed streams. Generally, sources for carbon dioxide as flue gases will be present and the stream needs to be separated, purified and pressurized in order to be used in the subsequent processes. The size of the carbon dioxide stream will define the scale of the hydrogen production. Table 26 provides an overview of the typical size of carbon dioxide streams from some potential carbon dioxide sources, the corresponding stoichiometric hydrogen streams for a given process and the corresponding product stream.

Table 26: Typical CO_2-sources and their respective stochiometric volume flows for Power-to-Gas and Power-to-Liquid applications[119,120]

CO_2-Source		Methanation		Methanol production		Fischer-Tropsch-fuels	
	volume flow m^3/h	**H_2-stream m^3/h**	**CH_4 m^3/h**	**H_2-stream m^3/h**	**CH_3OH t/h**	**H_2-stream m^3/h**	**$-CH_2-$ t/h**
Biogas plant	500	2,000	500	1.500	0.7	1.500	0.3
Gasification of biomass	2.100 (+1.400	8.400 (+4.200)	2.100 (+1.400)	6.300 (+2.800)	2.8 (+1.8)	6.300 (+2.800)	1.2 (+0.8)

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[118] EU ETS data 2015, http://www.eea.europa.eu/data-and-maps/data/data-viewers/emissions-trading-viewer-1

[119] Bajohr/Graf/Götz 2013; S. Bajohr, F. Graf, M. Götz, „Bewertung der Kopplung von PtG-Konzepten mit einer Biomassevergasung“, gfw-Gas, 4/2013, 222-226.

[120] Ausfelder et al. „Energiespeicher als Element einer sicheren Energieversorgung“; Chem. Ing. Tech. 2015, 87, No. 1–2, 17–89.

	CO)						
Ammonia plant	30,000	120,000	30,000	90,000	39	90,000	17
Coal-fired power station (500 MW, 930 g/kWh)	240,000	960,000	240,000	720,000	314	720,000	137

Standard conditions (298.15 K; 101,300 Pa); for comparison, a typical stack for alkaline electrolysis produces a volume flow of 740 m^3/h H_2.

7.2 Steel manufacturing as a sources of hydrogen, CO and CO_2/CO mixed streams

Steel manufacturing provides a source of hydrogen, carbon monoxide or CO_2/CO mixed streams which can be attractive for chemical valorization. A number of research projects have been started to explore such industrial symbiosis schemes. For instance, the Carbon2Chem project[121] aims at using emissions from steel production as raw material for chemicals.

60% of the steel in Europe is produced via the basic oxygen furnace (BOF) process. In a blast furnace (BF) pig iron is extracted from iron ore using coke. The formed blast furnace gas is usually used for generating electricity. The iron from the blast furnace is then further refined and converted to steel in the BOF. Depending on the plant, 20-30% of scrap is added to this process, primarily to regulate the temperature.

In this BF-BOF route, process gases are generated in the coke plant, the BF and the BOF converter. These off-gases are usually recovered and used to generate electricity and steam. European integrated steel mills therefore mostly include a power plant. The route avoids emissions of toxic CO, and allows for self-sufficiency of steel plants in terms of electricity. However, the power plants are rather inefficient and produce power at 30 and 40% efficiency compared to modern gas-fired power plants running at up to 60% efficiency.

Table 27 shows typical parameters of the steel production off-gases. BF gases by far comprise the highest volume flow, but BOF gases are particularly interesting due to the high concentration of CO. and the CP gas is characterized by high hydrogen contents. The availability of these gases from European steel production has been estimated using the listed concentrations and extrapolating based on the European production of crude steel via the oxygen route, which was 101 Mt in 2015[122]. The resulting numbers have subsequently been used to calculate the amount of methanol that could be produced with these gases.

It is evident, that off-gases from the steel industry would provide a large potential for chemical manufacturing. The hydrogen would suffice for 2 Mt methanol, corresponding to Europe's anticipated production volume in 2050 (only for chemicals, without methanol for low-carbon

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[121] https://www.thyssenkrupp.com/de/carbon2chem/

[122] World Steel Association, World steel in figures 2016.

pathways). CO actually has a very high use potential and would supply enough carbon for more than 50 Mt methanol p.a.

Table 27: Composition of steel production off-gases and potentials for chemical production

Steel production off-gases	CP	BF	BOF
Volume [m^3/t steel]	150	1500	75
CO [vol%]	6.8	22	70
Amount CO in Europe [Mt]	0.6	37.8	10.8
Equivalent to methanol [Mt]	**0.7**	**43**	**12.3**
H_2 [vol%]	61	2	1.5
Amount H_2 in Europe [Mt]	0.38	0.25	0.02
Equivalent to methanol [Mt]	2	1.3	0.1
CO_2 [vol%]	1.7	22	13.5
Amount CO_2 in Europe [Mt]	0.3	64.2	3.6
Equivalent to methanol [Mt]	0.2	47	2.6

It is quite obvious that electricity generation from process hydrogen in the steel industry on the one hand, and hydrogen production from electricity by the chemical industry on the other hand does not constitute the most efficient use of energy and feedstocks. Enlarging energy and feedstock streams beyond the battery limits of individual sectors can create substantial efficiency and CO_2 abatement potentials. However, it will be an enormous effort to define business models and contractual frameworks that would leverage such potentials. For instance, in the case of the depicted flue gas streams of the steel industry used for chemical production, a reasonable compensation for the additional electricity demand of the steel sector would need to be offered to the steel producer. It has also to be pointed out, that a stronger dependence between the sectors is created on the basis of such coupled productions, which doe not only entail advantages.

7.2.1 Use of steel manufacturing off-gases for ethanol production

A pathway utilising the CO from blast furnace gas to produce ethanol in a gas fermentation process using acetogenic microbes (*Clostridium autoethanogenum*) has been developed by

Lanzatech.[123] Using the subsequent ethanol conversion to ethylene described in chapter 6.3, this process could serve as an alternative pathway to ethylene.

The steel mill gas containing a mixture of CO, CO_2 and H_2 is cleaned and fed into a fermentation reactor, where it is converted into ethanol. The process has been demonstrated at pilot-scale (50-100 kg/day) since 2008 using waste flue gas streams from the BlueScope Steel mill in Glenbrook, New Zealand. A campaign in a 16 m^3 vessel (corresponding to 300 t/yr) has been realised with Baosteel in Shanghai. A second pre-commercial facility using steel mill waste gases is in operation near Beijing with Capital Steel.

ArcelorMittal has started a collaboration with Lanzatech in 2012, focusing on the ethanol productivity and upscaling of the technology for a 5 Mt integrated plant. Within the Steelanol project[124] a further upscaling step to realize a demonstration plant in the harbor of Ghent producing 47 kt of ethanol per year is targeted. This will bring the technology from TRL 5 to 7.

LanzaTech’s proprietary microbes are able to compensate for a deficiency in hydrogen by utilising a biological water gas shift reaction within the microbe, which allows the process to run on hydrogen-free CO gas streams.[125] The stoichiometry for the formation of ethanol from CO and water in this case is as follows:

$$6\,CO + 3\,H_2O \rightarrow CH_3CH_2OH + 4\,CO_2$$

With CO as sole substrate carbon source, one third of the carbon from CO can be converted to ethanol, with the remaining two thirds being released as CO_2. Ethanol production is increased, however, with increasing availability of hydrogen. Theoretically, in a fermentation substrate gas containing CO and H_2 in a ratio of 1:1, two thirds of the CO can be converted to ethanol as given below:

$$6\,H_2 + 6\,CO \rightarrow CH_3CH_2OH + 2\,CO_2$$

Table 28 summarizes the stoichiometric demand for CO and hydrogen as well as the corresponding emissions from CO_2 generated in the fermentation process.

Table 28: Steelanol process: Stoichiometric demand for CO and H_2 and corresponding CO_2 generated in the fermentation process

Gas mixture	CO demand [t/t ethanol]	Hydrogen demand [t/t ethanol]	CO_2 generated [t/t ethanol]
CO only	3.65	0	3.82
CO/H_2 1:1	3.65	0.263	1.91

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[123] Technical background on the LanzaTech Process, http://www.arpae-summit.com/paperclip/exhibitor_docs/14AE/LanzaTech_Inc._131.pdf

[124] http://www.steelanol.eu/

[125] Microbial fermentation of gaseous substrates to produce alcohols, WO 2007117157 A1

A recent life cycle assessment[126] has investigated different process configurations for gas fermentation to ethanol, including the use of BOF gas. The LCA shows net GHG emissions of 31.4 gCO_2eq/MJ ethanol or 0.84 tCO_2eq/t ethanol (well-to-wheel), which corresponds to a 67% emission reduction compared to gasoline. However, the LCA assumes that the BOF gas utilised in the process would have been flared otherwise, with oxidation of all carbon to CO_2, before being released to the atmosphere. The authors argue, that about 25% of all BOF steel mill gases are flared in Europe, instead of being used for heat or power generation, and that the percentage is much higher globally. Nevertheless a full credit in substitution of flaring is not considered as valid in case of European steel mills, in which BOF gas is utilised to a large extent. In the mentioned LCA, a credit of 1.19 t CO_2/ton BOF gas has been allocated to the process, based on a carbon content of 324 kg C per ton BOF gas. The net credit of GHG emissions avoided by not flaring the BOF gas combined with the GHG emissions of the vent gas released from the bioreactor corresponds to 2.12 tCO_2eq/t ethanol. If this net credit is not taken into account, the resulting carbon footprint of the produced ethanol is not favourable anymore. This illustrates the need for LCAs with appropriate methodology and boundary conditions including existing valorisation of streams considered as alternative feedstock.

7.3 Other industrial symbiosis opportunities

The industrial symbiosis elements described in this study only concern selected synergies which can be considered as obvious in terms of the scope of this study. Other waste gas streams from refineries, biogas plants and waste incineration plants can be considered as well in this regard. Moreover, cross-sectorial and even industrial–municipal use of waste heat and water also constitute important industrial symbiosis elements, but has not been taken into account here.

8 Recycling and polymer waste as feedstock for the chemical industry

As part of the concept of circular economy, the impact of recycling of polymers and polymer waste as feedstock is considered. The use of these "secondary raw materials" can be less energy-demanding than the de novo synthesis and reduces the amount of primary feedstocks.
A study provided by Accenture [127] describes the potential for an industrial transition towards a circular economy, in which chemical industry products and materials are recycled and reused. The concept of "circulating molecules" as entitled by Accenture, encompasses five

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[126] R. M. Handler, D. R. Shonnard,E. M. Griffing, A. Lai, I. Palou-Rivera, Life Cycle Assessments of Ethanol Production via Gas Fermentation: Anticipated Greenhouse Gas Emissions for Cellulosic and Waste Gas Feedstocks; Ind. Eng. Chem. Res. 2016, 55, 3253−3261.

[127] Accenture, Taking the European Chemical Industry into the Circular Economy, https://www.accenture.com/us-en/insight-circular-economy-european-chemical-industry

recirculating loops, which would enable up to 70 percent of the molecules provided by the European chemical industry to be recirculated, according to Accenture's estimate:

- Loop 1: Circularity based on renewable feedstock
- Loop 2: Circularity based on increased reuse of products containing chemical-industry outputs
- Loop 3: Circularity based on molecule reuse (mechanical recycling)
- Loop 4: Circularity based on modification of molecules and reuse of precursors (chemical recycling)
- Loop 5: Circularity based on energy recovery and reuse of CO_2

Loop 1 has essentially been covered by this study. As for the other loops 2-5, the order they are presented here clearly describe a hierarchy of preferred options.

Direct reuse of chemical products (loop 2), such as the already practiced reuse of PET bottles, is obviously preferable over the subsequent options. Accenture estimates that 18% (19 Mt) of the total chemical products can be reused. This loop effectively reduces the demand for of new polymer products, production volumes would decrease accordingly (anticipated production volume of ethylene and propylene in 2050 is at 33.5 and 17 Mt respectively).

Loop 3 entails the reuse of materials rather than products. An example is the reuse of plastic materials from automobiles and packaging. This requires substantial logistic and technical infrastructure for collection, sorting, cleaning, and re-processing of reused materials. Accenture estimates a potential of 28% (30 Mt) of the European chemical products, but also points out the requirement of 18 Mtoe of energy for the recycling process, 34% of today's energy consumption of the European chemical industry.

Loop 4, chemical recycling, entails the use of chemical products as secondary raw materials, thereby substituting other feedstock. Catalytic cracking and plasma gasification has been mentioned as key technologies by Accenture in this respect, and a long term potential of 10 Mt of molecules has been anticipated.

Loop 5 refers to the combustion of waste plastics for energy recovery and utilisation of the generated CO_2. In this respect, this study covers part of the loop 5 aspects. Accenture estimates a recirculation of 9 Mt of molecules this way.

Table 29 summarizes the assumptions provided by Accenture. The energy demand for the different recycling loops provided by Accenture can be compared to the energy demand for producing corresponding amounts of polymers “de novo”, using the low-carbon synthesis routes (via hydrogen and CO_2) described in this study. As the last column in Table 29 shows, recycling of polymers, while consuming energy, still is advantageous in terms of energy consumption compared to de novo synthesis. The corresponding reduction in energy demand is a result of lower de novo production due to product reuse and reduced energy demand for the process based on recycle raw materials. In accordance with a low-carbon production scenario the energy consumption of the hydrogen/CO_2 based route has been used for the calculations.

Table 29: Impact of recycling (recirculating) loops as anticipated by Accenture and corresponding impact on low-carbon production of ethylene and propylene and related energy consumption*

Loop	Accenture estimate of volume potential and energy requirement[127]	Corresponding reduced production of olefins in 2050	Reduced energy demand for olefins*
Reuse of products	18% reuse, 19Mt	18% of olefins: 9Mt	20.8 Mtoe
Molecule reuse (mechanical recycling)	5 Mt of plastics currently, could rise to 29.5 Mt (28 % of the total chemicals output); collection, sorting, cleaning, and re-processing requires 18Mtoe	28% of olefins: 14Mt	23 Mtoe
Modification of molecules and reuse of precursors (chemical recycling)	catalytic cracking and plasma gasification, 9.6 Mt (9 % of the total chemicals output); requires 4 Mtoe	9% of olefins: 4.5Mt	8 Mtoe
Energy recovery and reuse of CO_2	9 Mt (8.5 % of the total chemicals output); requires 9 Mtoe	8.5% of olefins: 4.3Mt	5.3 Mtoe
*calculated as energy demand for de novo synthesis (CO_2/H_2 route) - energy demand for recycling		***Total:***	57.1 Mtoe

The total energy saving would amount to 57.1 Mtoe or 663 TWh of low-carbon electricity. The impact on CO_2 emissions have not been quantified in the Accenture study. Recycling of polymer waste streams has therefore not been integrated in the CO_2 emission reduction scenarios of this study. A thorough life cycle investigation of the individual recirculating loops would be required, including the energy demand and carbon footprint of collection logistics, sorting, cleaning and reprocessing for specific products or value chains.

This study focuses on de novo processes. Higher recycling rates would of course impact the overall conclusions of this study, as they would have a direct effect on the demand for de novo polymers, hence a reduction of demand for monomers and precursors such as methanol. Future investigations should combine the two aspects of low carbon de novo synthesis and different recycling options. In addition, a comparison with alternative use options, such as energy recovery in municipal waste incineration or use as secondary fuel in the cement industry should also be considered.

9 Scenarios describing a low-carbon chemical industry

The previous chapters have provided the data basis for the subsequent scenario work. As a reminder it has to be emphasized that the following scenarios do not necessarily reflect a future reality, they merely describe the corridor of possible impact In terms of quantitative CO_2 reduction potentials, energy and feedstock demand, as well as investments and production cost based on a large number of assumptions. The different scenarios and basic assumptions have been described in chapters 1.2.3 and 1.3. Other assumptions, such as ambitions for the implementation of certain technology pathways are described in this chapter. Annex 2 provides an overview on the ambitions for all scenarios.

9.1 Business as usual

The **business-as-usual scenario (BAU)** extrapolates the current (2015) status of the chemical industry in terms of energy demand and GHG emissions into the future, thereby assuming no further improvements whatsoever in any of these categories via implementation of new technology options and advancement of efficiency measures. In this sense the BAU scenario assumes a “freeze” of the current state of the art and impact is exclusively a function of changing production volumes. This deliberately set baseline obviously does not reflect the reality, which is, that the European chemical industry is continuously improving energy efficiency of existing production assets. The BAU scenario only refers to the chemical industry with regard to the 9 large volume products investigated. The fuel sector is not covered here, as the chemical industry does not offer low-carbon opportunities to the transport sector under the BAU scenario.

9.1.1 Volume of chemical production

As a basic assumption this study assumes a continuous supply of products and materials by the European chemical industry with a 1 % growth per annum. Regional changes in chemicals production or shift of production to other world regions outside Europe (delocalization) are not considered in the scope of the study. The anticipated production volumes of the 9 large chemicals plus urea investigated based on this assumption are provided in Figure 16, showing a steady increase in production from a total volume of 100 Mt in 2015 to 140 Mt in 2050.

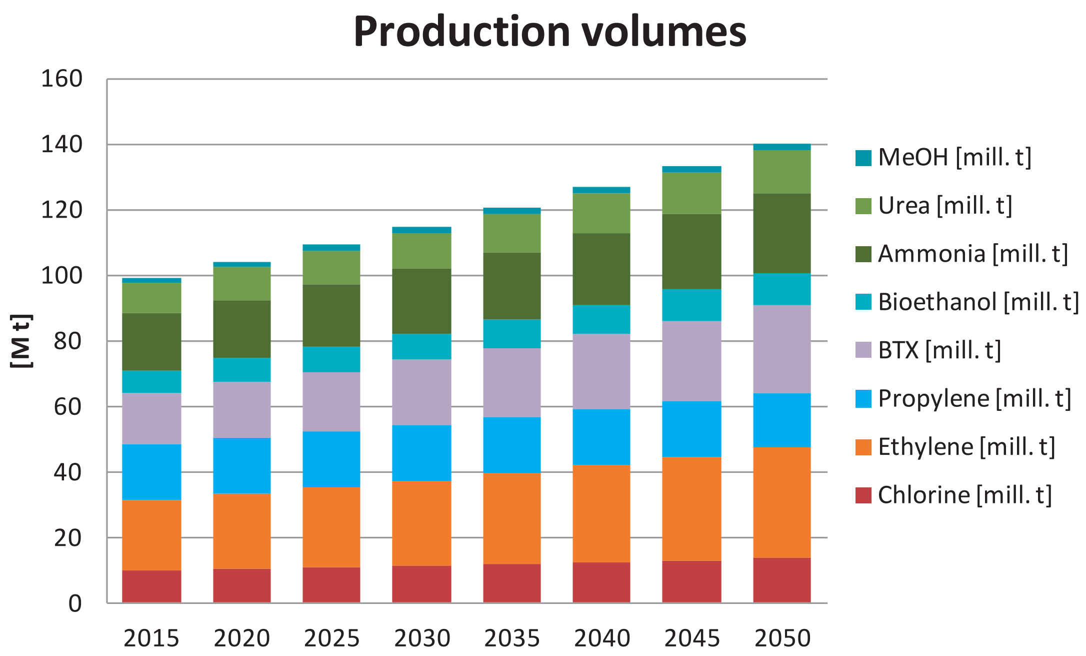


Figure 16: Anticipated production volumes of 9 large volume chemicals including urea in Europe

9.1.2 CO_2 emissions BAU

Figure 17 depicts the corresponding CO_2 emissions assuming emission factors as of today. As expected, emissions will increase proportional to production volumes, from 85 to 119. In order to keep a consistent BAU picture it has also been assumed that the power sector does not show further progress in decarbonization, hence the same emission increase for the chlorine production as the only already electricity-based process.

As already discussed in the introduction of this chapter, efficiency measures are not included in the BAU scenario. It is to be pointed out again, that this BAU baseline scenario does not consider the ongoing efforts of the chemical industry in reducing energy intensity of existing production plants. If energy efficiency measures, as discussed in chapter 2.5, are taken into account in a “BAU scenario including energy efficiency”, the BAU CO_2 emissions have to be reduced by the numbers shown in Table 30.

Table 30: Impact of efficiency measures on CO_2 emissions in a “BAU scenario including energy efficiency”

Impact of efficiency measures	2015	2020	2025	2030	2035	2040	2045	2050
Reduced CO_2 emissions [Mt CO_2eq]	-	1.93	3.86	5.71	7.55	9.60	11.88	14.34

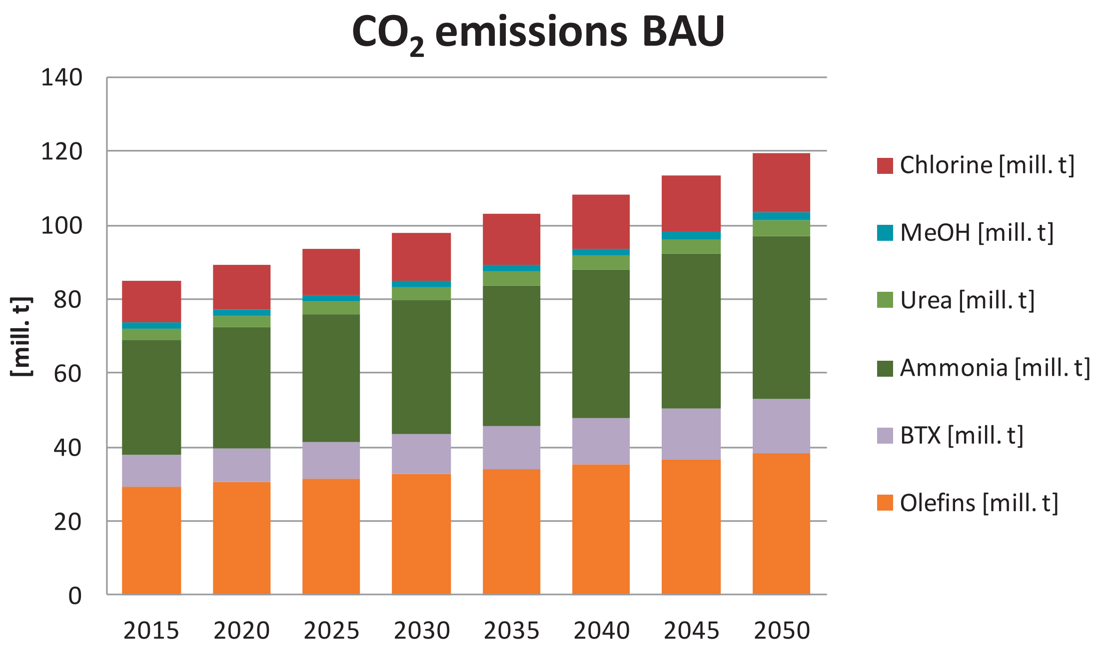


Figure 17: CO_2 emissions under the BAU scenario.

9.2 Maximum scenario

The maximum scenario depicts the upper limit assuming 100% deployment of all new technologies described in the previous chapters. As hydrogen and biomass-based processes are competitive, an arbitrary share of the booth pathways has been assumed. Hydrogen based pathways have been favoured in volume due to the stronger CO_2 avoidance potentials and concerns about the limited availability of biomass (see chapter 6.7). Together, the hydrogen and biomass pathway yield 100% of the production in 2050. This is the case for methanol and olefin production, but also the share of methanol in gasoline and the bioethanol share are complementary and add up to 100%.

In order to achieve this, a 2.85% p.a. replacement rate of existing chemical production capacities has been assumed, which results in 100% new production facilities by 2050. Likewise, deployment of electric steam generation and steam re-compression is considered to progress strongly beyond 2025 to reach 100% in 2050.

Assumptions for the maximum potential are summarized in Table 31.

Table 31: Assumptions for the max scenario

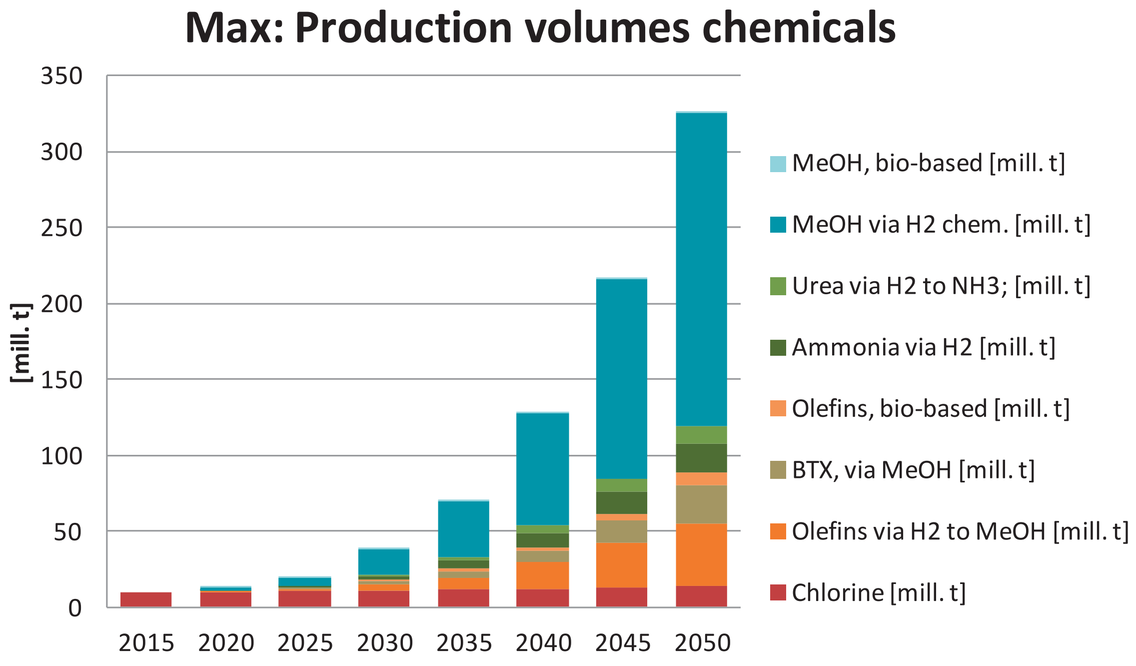
Assumptions	2015	2020	2025	2030	2035	2040	2045	2050
Share of H_2-based MeOH plants	0%	5%	10%	20%	40%	60%	75%	85%
Share MeOH in gasoline	0%	5%	10%	20%	30%	45%	70%	96.5%

Share syn. Jetfuels	0%	5%	10%	20%	30%	45%	70%	100%
Share syndiesel	0%	5%	10%	20%	30%	45%	70%	100%
Share bioethanol	0%	0.6%	0.8%	1.0%	1.3%	1.8%	2.7%	3.5%
Share olefins via H_2-based MeOH	0%	5%	10%	20%	30%	50%	70%	85%
Share BTX via H_2-based MeOH	0%	5%	10%	20%	30%	45%	70%	100%
Share biomass based MeOH	0%	1%	2%	3%	4%	5%	10%	15%
Share biomass based olefins	0%	1%	2%	3%	4%	5%	10%	15%
Plant replacement rate	2.85% p.a.				100% in 2050			
	0%	14%	29%	43%	57%	71%	86%	100%
Electric steam generation and steam recompression	0%	2%	5%	15%	30%	50%	70%	100%
Efficiency measures	0.56% p.a.							

9.2.1 Max scenario: production volumes

Resulting production volumes based on these assumptions are depicted in Figure 18, for both chemical production only (Figure 18 a) and corresponding production volumes including the fuels (grey lines in Table 31).

a)



b)

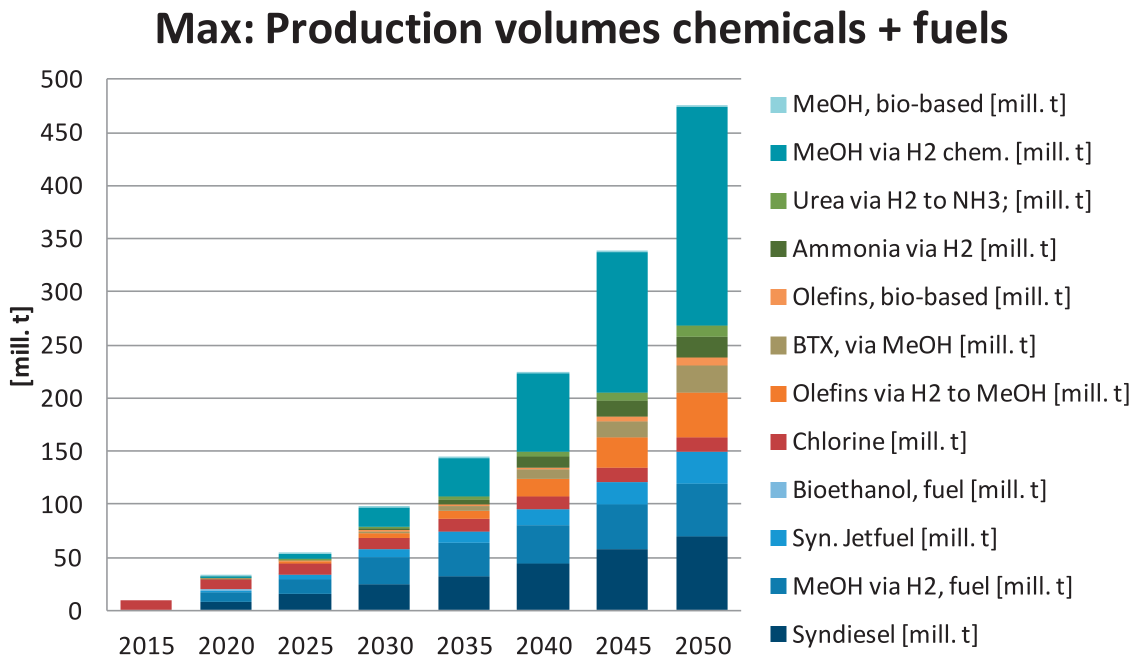


Figure 18: Production volumes max scenario; a) chemicals only b) chemicals and fuels

A very dominant factor in the production volumes under the max scenario is the high amount of low-carbon methanol production for chemicals, due to the fact, that the scenario foresees the production of the main share of ethylene and propylene and all BTX via methanol.

The production of synthetic fuels seems relatively low with 150 Mt in total, compared to the chemicals production. The reason for this is the strong reduction of transport fuels foreseen in the IEA ETP2015 2°C scenario. For diesel, gasoline and jetfuels, the total consumption is expected to decrease from 14000 PJ today to 5300 PJ in 2050.

9.2.2 Max scenario: CO_2 emission reduction

Figure 19 depicts the maximum CO_2 emission reduction potential of the technologies described in this study. For the chemical industry (Figure 19a) the potential CO_2 emission reduction amounts to 210 Mt in 2050, which would actually exceed the emissions under the BAU scenario by 76%. This is due to the negative carbon footprint for some of the products, in which CO_2 or biomass is built in. For synthetic fuels, the potential is even higher and amounts to 288 Mt. Combined, the potential impact on chemicals and fuels is at 498 Mt, 420% of the chemical sector's own BAU emissions in 2050.

The impact of energy efficiency measures is extremely low under this scenario, as total substitution of existing plant capacities is envisioned. Electricity based steam has an impact of 20 Mt in 2050.

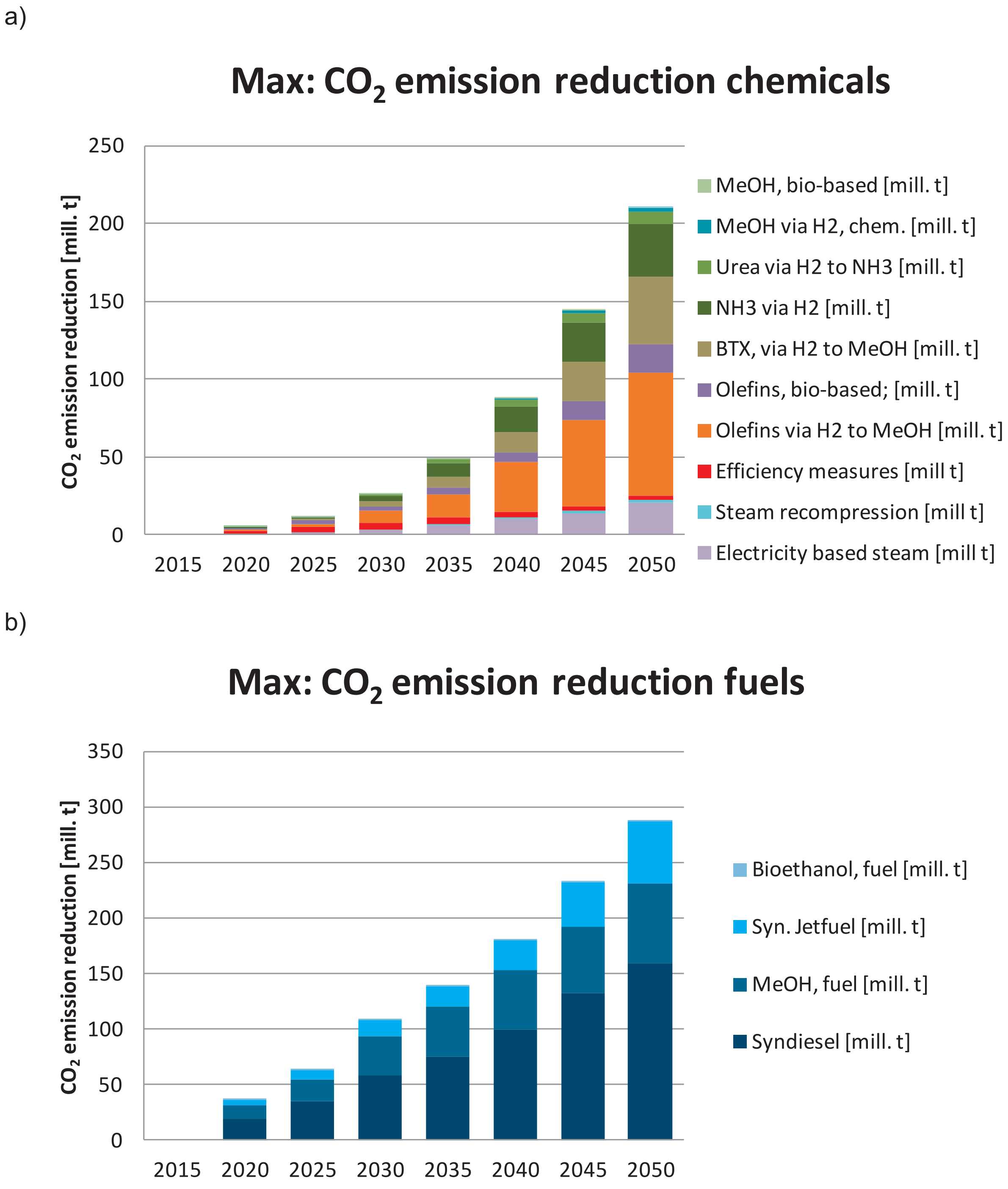


Figure 19: CO_2 reduction potentials under the Max scenario: a) chemical, b) fuels

Energy and resource requirements such as CO_2 and biomass demand are discussed in chapter 10 for all scenarios, as this facilitates the comparison of the impact of the different ambitions.

9.3 Intermediate scenario

The intermediate scenario (Interm) assumes continuous improvements of process efficiencies by efficiency measures and a slow starting, but steadily increasing deployment of breakthrough technologies. Steam generation by electricity and steam re-compression are implemented at full scale by 2050, as these technologies are relatively easy to implement and also are economically viable under current framework conditions. Energy efficiency measures are continuously implemented in existing plants via retrofits and optimizations. Policy measures will be required supporting an increasing biofuel quota which would also include synthetic fuels from CO_2. For chemical production, policy measures have to be in place to incentivize investments and to close the economic gap compared to the established fossil feedstock based processes. A 1% p.a. replacement rate of existing chemical production capacities has been assumed, which results in 35% new production facilities by 2050. In summary this scenario is not to be considered as easy to achieve. It already includes ambitious targets, e.g. in terms of plant replacement rates, that exceed the current level.

Table 32 summarizes the assumptions for the intermediate scenario, which are still ambitious, despite being the most conservative of the scenarios depicted in this study.

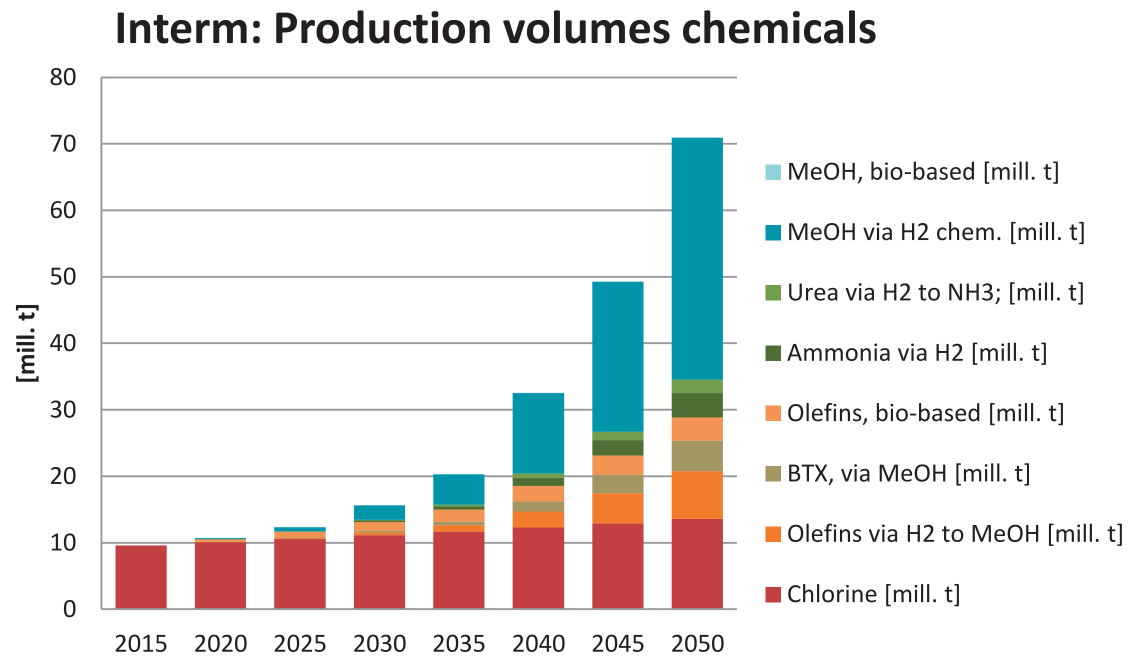
Table 32: Assumptions for the interm scenario

Assumptions Interm	2015	2020	2025	2030	2035	2040	2045	2050
Share of H_2-based MeOH plants	0%	1%	2.5%	5%	7.5%	15%	23%	30%
Share MeOH in gasoline	0%	1%	2.5%	5%	7.5%	10%	15%	20%
Share syn. Jetfuels	0%	0.5%	1.0%	2.5%	5%	7.5%	10%	15%
Share syndiesel	0%	0.5%	1.0%	2.5%	5%	7.5%	10%	15%
Share bioethanol	0%	0.6%	0.8%	1%	1.3%	1.8%	2.7%	3.5%
Share olefins via H_2-based MeOH	0%	1%	3%	5%	8%	15%	23%	30%
Share BTX via H_2-based MeOH	0%	1%	3%	5%	8%	15%	23%	30%
Share biomass based MeOH	0%	1%	2%	3%	4%	5%	5%	5%
Share biomass based olefins	0%	1%	2%	3%	4%	5%	6%	7%
Plant replacement rate	1% p.a.				35% in 2050			
	0%	5%	10%	15%	20%	25%	30%	35%
Electric steam generation and steam recompression	0%	2%	5%	15%	30%	50%	70%	100%
Efficiency measures	0.56% p.a.							

9.3.1 Intermediate scenario: low-carbon production volumes

Resulting production volumes based on these assumptions are depicted in Figure 20, for both chemical production only (Figure 20 a) and corresponding low-carbon production volumes including fuels (Figure 20 b, grey lines in Table 32).

a)



b)

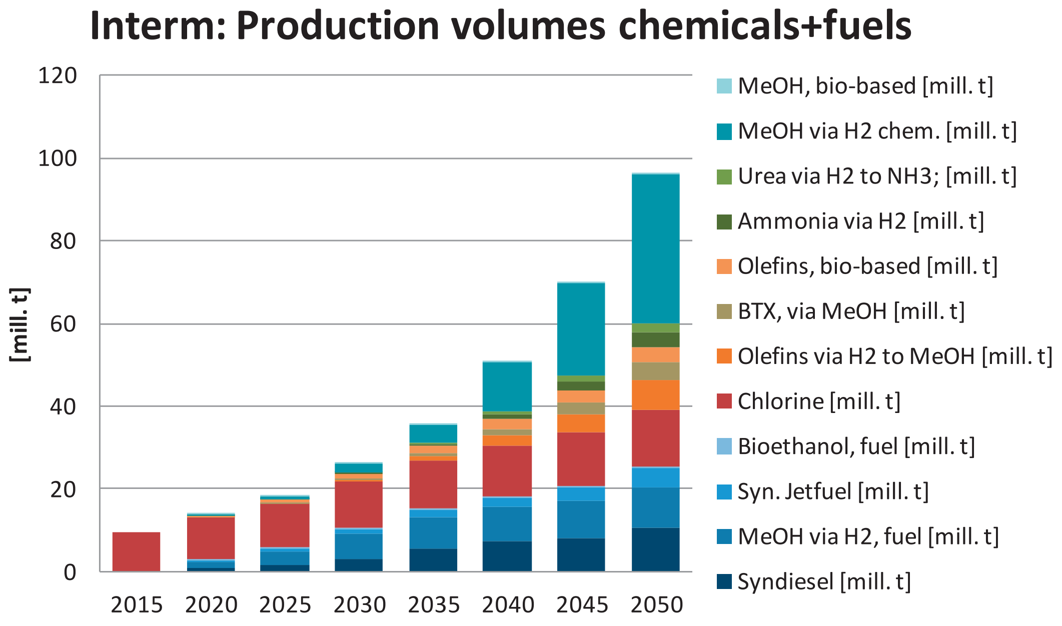


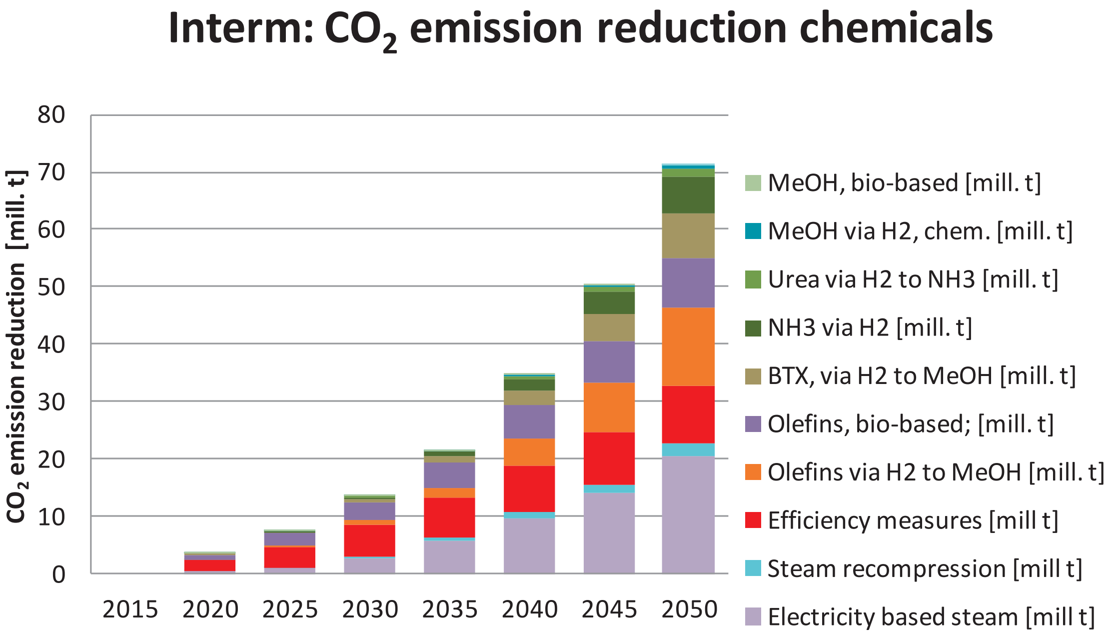
Figure 20: a) Low carbon production volumes interm scenario; a) chemicals only b) chemicals and fuels

Production volumes in Figure 20 only show the low-carbon production technologies. Remaining production demand as depicted in the BAU is still to be covered by the fossil feedstock based processes. As in the max scenario, the production volumes of low-carbon methanol production are strongly increasing, as methanol is the basis for low-carbon ethylene and propylene and BTX production via methanol, achieving 30% of the total production of these chemicals in 2050. Chlorine has a large part of the production volumes already today, as the total chlorine production is included and no technology change is required. Synthetic fuel production is still relatively moderate in the interm scenario.

9.3.2 Intermediate scenario: CO_2 emission reduction

Figure 21 shows the CO_2 emission reduction potential under the intermediate scenario. For the chemical industry, the CO_2 emission reduction amounts to 70 Mt, which would roughly correspond to a 59% decrease of the CO_2 emissions of the chemical industry expected in 2050. Electricity-based steam has a large impact in this scenario, as full deployment is already foreseen in the intermediate scenario. In total, ambitions depicted in Table 32 are not sufficient to achieve the CO_2 abatement target of 80 to 95% of CO_2 emissions for the chemical sector in Europe by 2050. For synthetic fuels 47 Mt emission reductions are achieved under the Interm. scenario, Combined,117 Mt emission reductions are achieved, 98% of the chemical sector's own emissions under the BAU scenario.

a)



b)

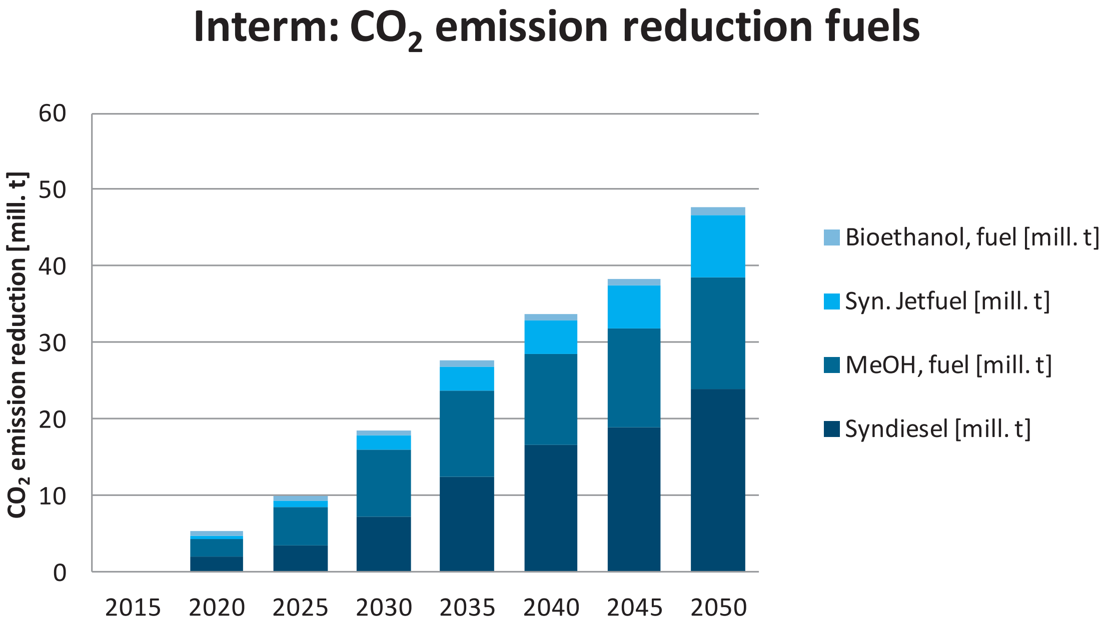


Figure 21: CO_2 reduction potentials under the Interm scenario: a) chemicals, b) fuels

Energy and resource requirements such as CO_2 and biomass demand are discussed in chapter 10 for all scenarios, as this facilitates the comparison of the impact of the different ambitions.

9.4 Ambitious scenario

The **Ambitious (Amb)** scenario is considered as very ambitious, but is well below the maximum potential. The share of low-carbon chemical production is increased to achieve 50% in 2050 which requires strong societal and policy support including financial incentives for favouring the substitution of fossil feedstock, high enough to make low-carbon technologies economically competitive and secure enough to stimulate large investments in these technologies. The share of renewable (including CO_2-based) fuels increases to 40%, by 2050, supported by an adequate fuel directive again leveraging the necessary incentives for both fuel producers and consumers. Energy efficiency measures are implemented and electrical steam generation and recuperation is fully deployed by 2050. The replacement rate of old plants has been increased from 1% to 1.5% p.a. which results in a 50% substitution of old plants by BPT level production plants. Realisation of lighthouse demonstration projects at around 5000t/a scale is strived for without delay, supported by efficient research and innovation efforts. Strategic alliances with other process industries are built to valorize industrial symbiosis potentials. Table 33 summarizes the ambitions assumed for the Amb scenario.

Table 33: Assumptions for the Amb scenario

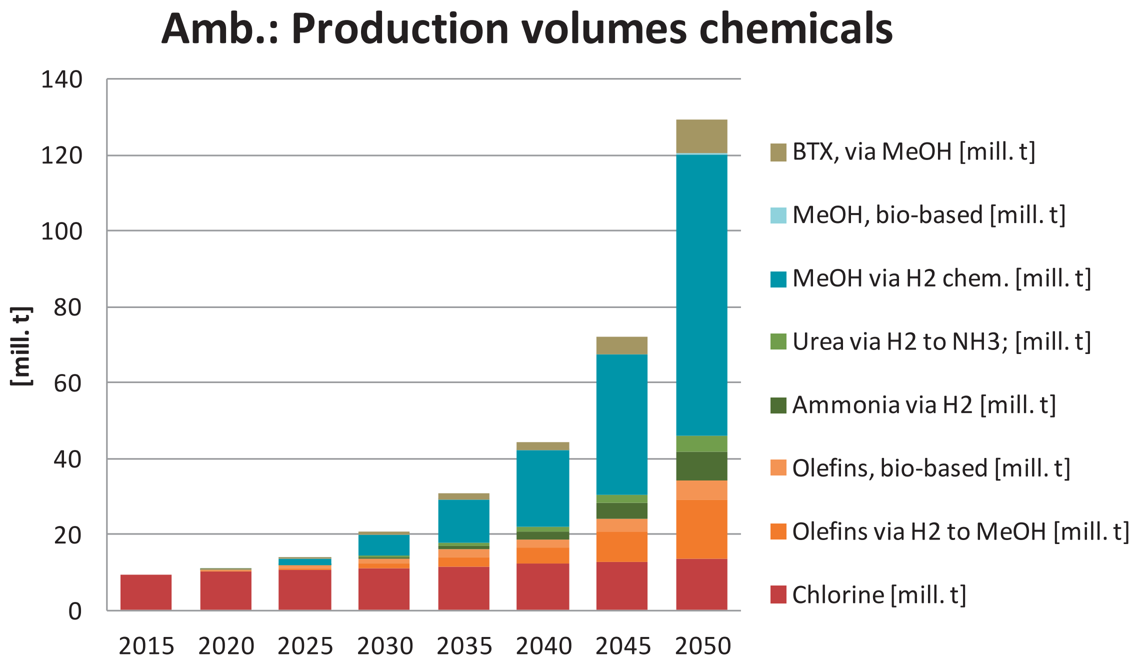
Assumptions Amb	2015	2020	2025	2030	2035	2040	2045	2050
Share of H_2-based MeOH plants	0%	1%	5%	10%	15%	20%	30%	50%
Share MeOH in gasoline	0%	1%	5%	10%	15%	20%	30%	36.5%
Share syn. Jetfuels	0%	1%	5%	10%	15%	20%	30%	40%
Share syndiesel	0%	1%	5%	10%	15%	20%	30%	40%
Share bioethanol	0%	0.6%	0.8%	1%	1.3%	1.8%	2.7%	3.5%
Share olefins via H_2-based MeOH	0%	1%	5%	10%	15%	20%	30%	50%
Share BTX via H_2-based MeOH	0%	1%	5%	10%	15%	20%	30%	50%
Share biomass based MeOH	0%	1%	2%	3%	4%	5%	7.5%	10%
Share biomass based olefins	0%	1%	2%	3%	4%	5%	7.5%	10%
Plant replacement rate	1.5% p.a.				53% in 2050			
	0%	8%	0%	8%	0%	8%	0%	8%
Electric steam generation and steam recompression	0%	2%	5%	15%	30%	50%	70%	100%
Efficiency measures	0.56% p.a.							

9.4.1 Ambitious scenario: low-carbon production volumes

Resulting production volumes based on these assumptions are depicted in Figure 22, for both chemical production only (Figure 22Figure 21 a) and corresponding production volumes including the fuels (Figure 22 b, grey lines in Table 33).

Production volumes in Figure 22 only show the low-carbon production technologies. Remaining production demand as depicted in the BAU is still to be covered by the fossil feedstock based processes. As in the max scenario, the production volumes of low-carbon methanol production are very high, at 74 Mt, supplying the feedstock for low-carbon ethylene, propylene and BTX production. Total chemical production is at 130 Mt in 2050. Fuel production is at 60 Mt in 2050 in this scenario.

a)



b)

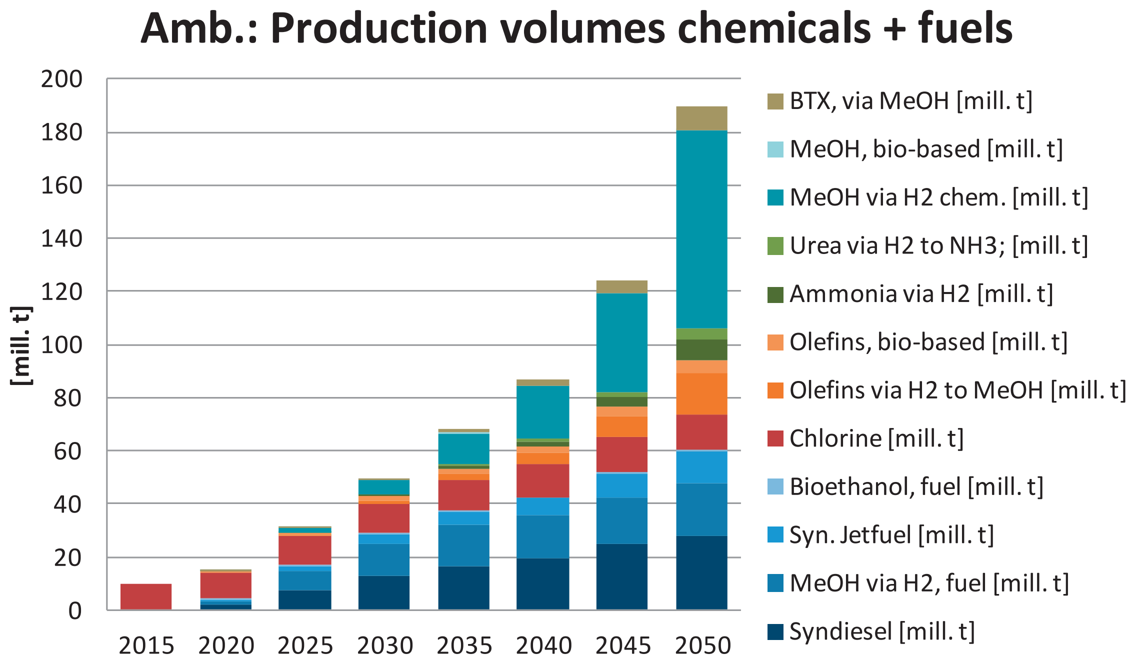
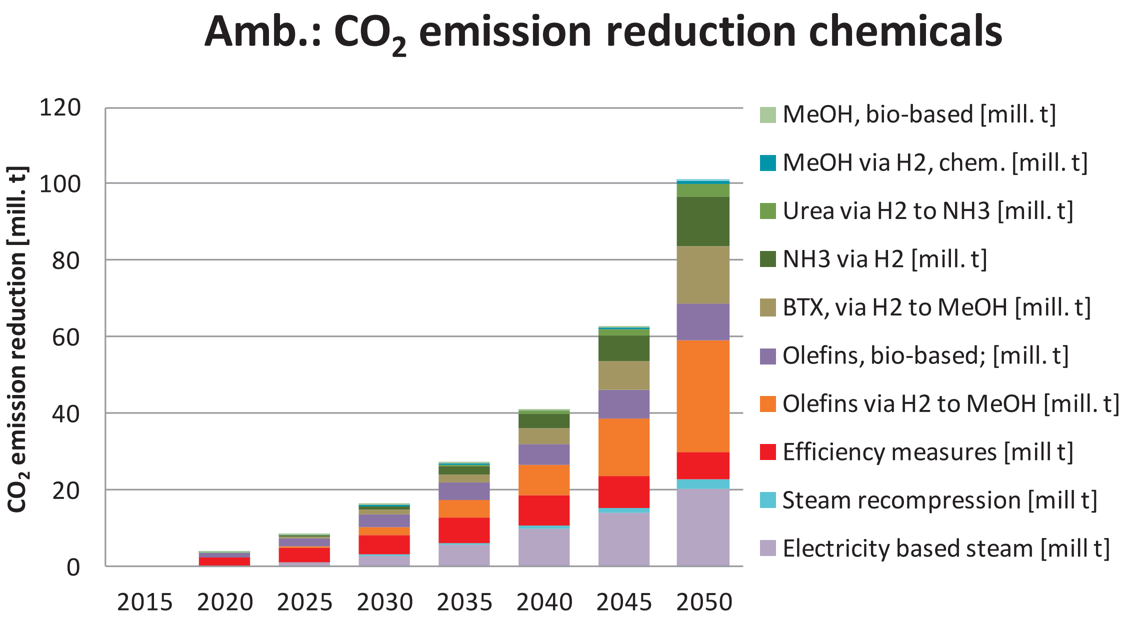


Figure 22: a) Low-carbon production volumes Amb scenario; a) chemicals only b) chemicals and fuels

9.4.2 Ambitious scenario: CO_2 emission reduction

Figure 23 shows the CO_2 emission reduction potential under the Amb scenario. For the chemical industry only (Figure 23 a) the CO_2 emission reductions amount to 101 Mt in 2050, corresponding to 84% of the emissions under the BAU scenario. This is in the range of the abatement target of 80 to 95% of CO_2 emissions for the chemical sector in Europe by 2050.

a)



b)

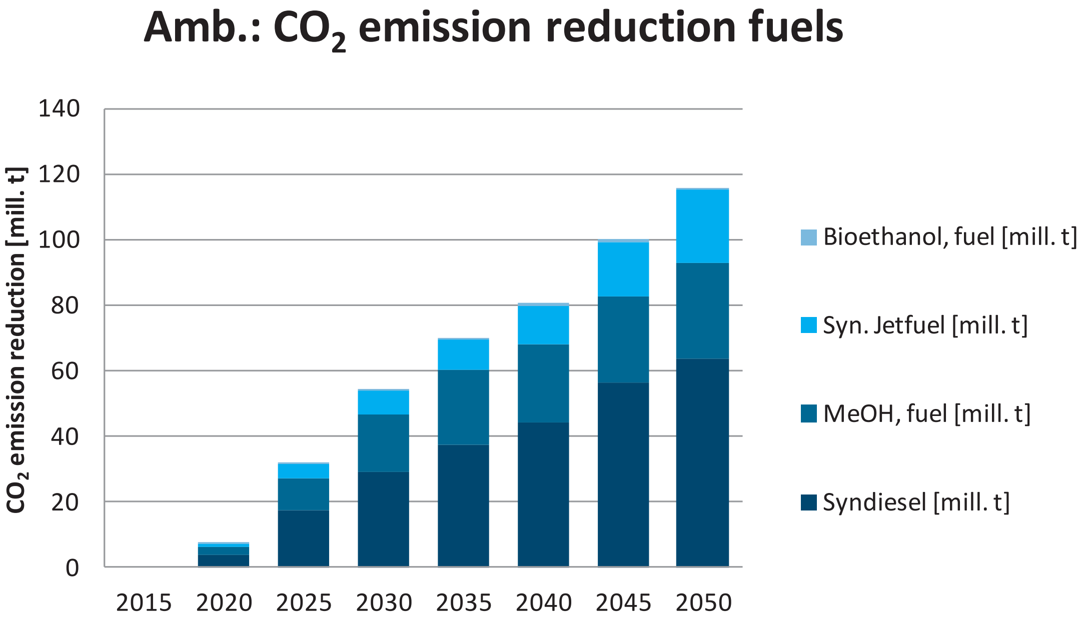


Figure 23: CO_2 reduction potentials under the Ambitious scenario: a) chemicals, b) fuels

For fuels (Figure 23 b) 115 Mt emission reductions are achieved. Combined, the potential emission reductions are at 216 Mt, 80% above the chemical sector's BAU emissions in 2050.

The impact of energy efficiency measures is lower compared to the intermediate scenario, as a relatively large share of plants is replaced by low-carbon technologies rather than refurbished. Electricity based steam remains at an impact of 20 Mt in 2050.

Energy and resource requirements such as CO_2 and biomass demand are discussed in chapter 10 for all scenarios, as this facilitates the comparison of the impact of the different ambitions.

9.5 Summary production volumes and CO_2 reduction potentials for the scenarios

Before the impact of the ambitions of the three scenarios Max, Amb and Interm is compared in terms of energy and feedstock demand, the results of chapter 9 are briefly summarized in overview figures. Figure 24 depicts the low-carbon production for the three scenarios.

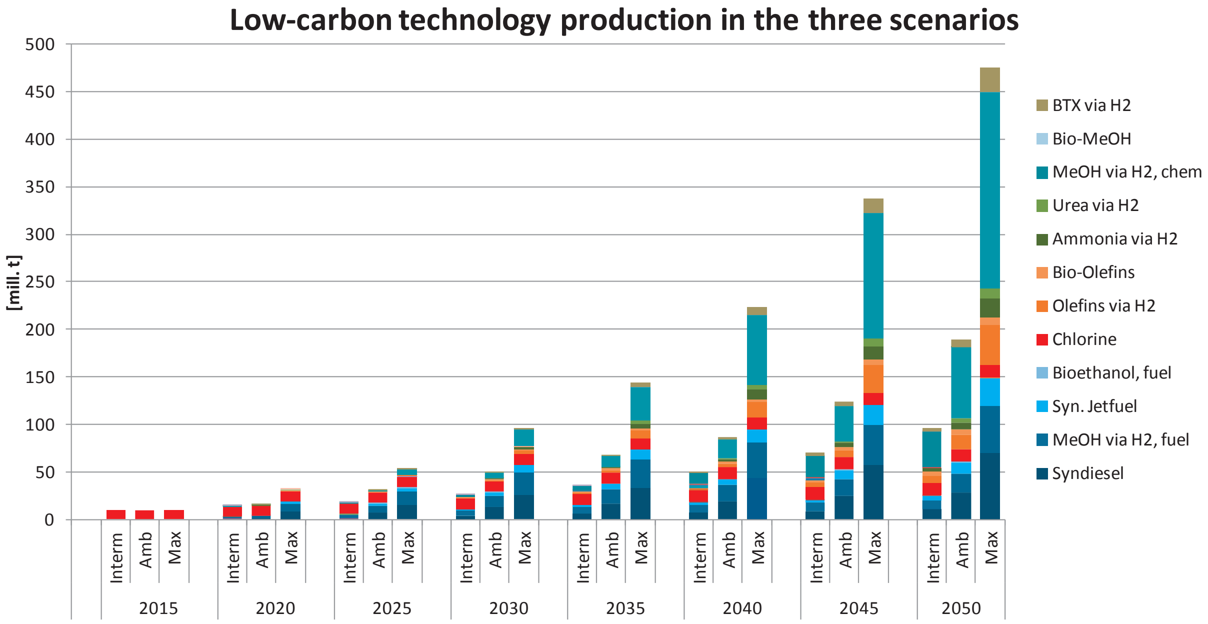


Figure 24: Production volumes based on low carbon technologies, all scenarios

The CO_2 emission reduction potentials are summarized in Figure 25 for both chemical production excluding and including fuels. Comparing the two cases indicates the relatively stronger impact of the fuels, which is driven by the relatively lower emissions compared to the fossil fuels they replace. It is reminded that CO_2 emission reductions for fuels are based on well-to-wheel emissions, hence including the use phase. This is different for the chemicals, for which only production (including feedstock production) is considered.

Additional impacts of a circular economy (chapter 8) can be expected, but could not be quantified due to the lack of carbon footprint data of the different recycling concepts or loops as described in chapter 8. For industrial symbiosis (chapter 7), specific scenarios need to be investigated that allow the assessment of the CO_2 footprint of the waste gas streams, for instance in terms of purification demand prior to chemical conversion.

a)

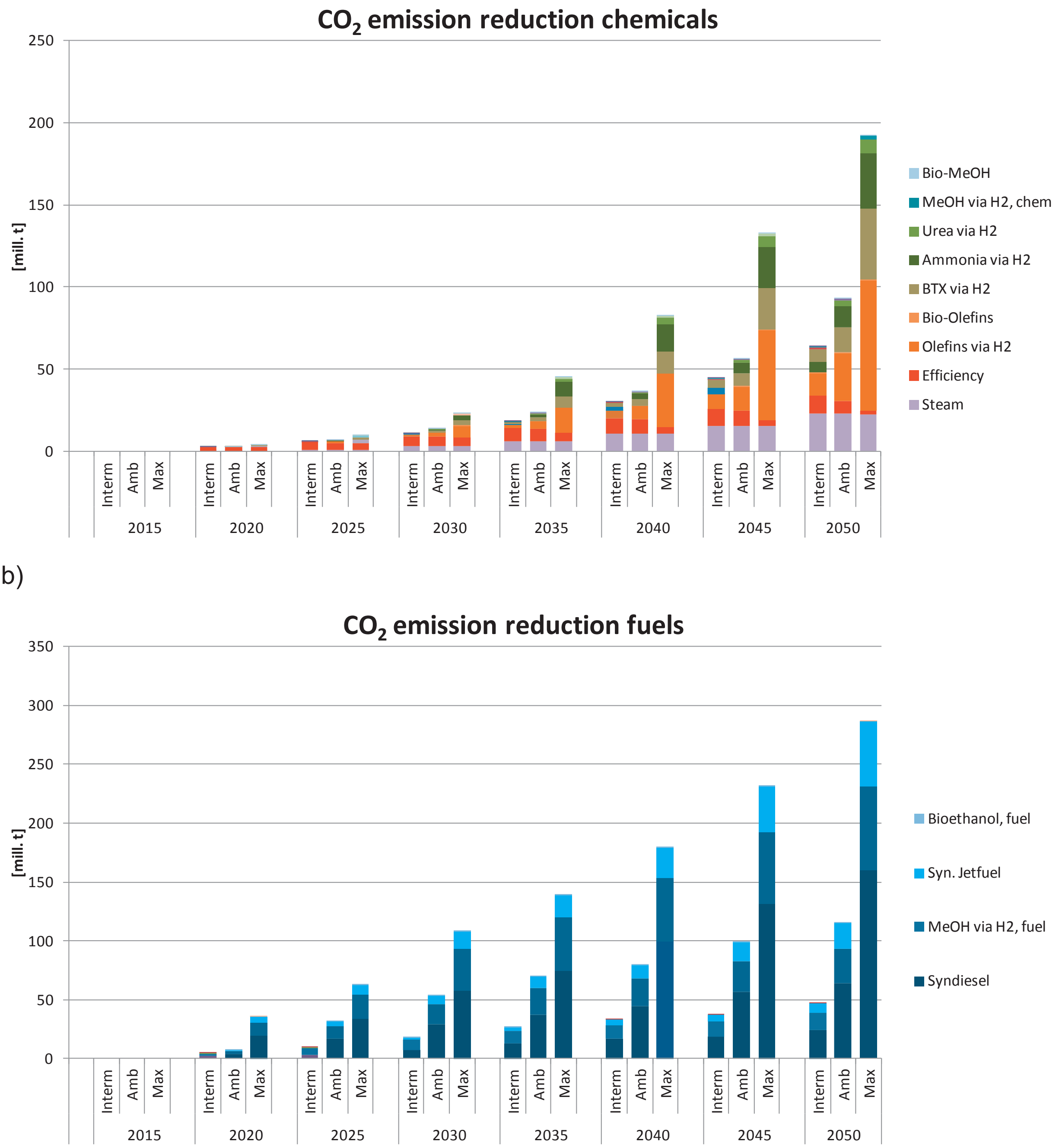


Figure 25: CO_2 emission reductions for all scenarios; a) chemicals; b) fuels

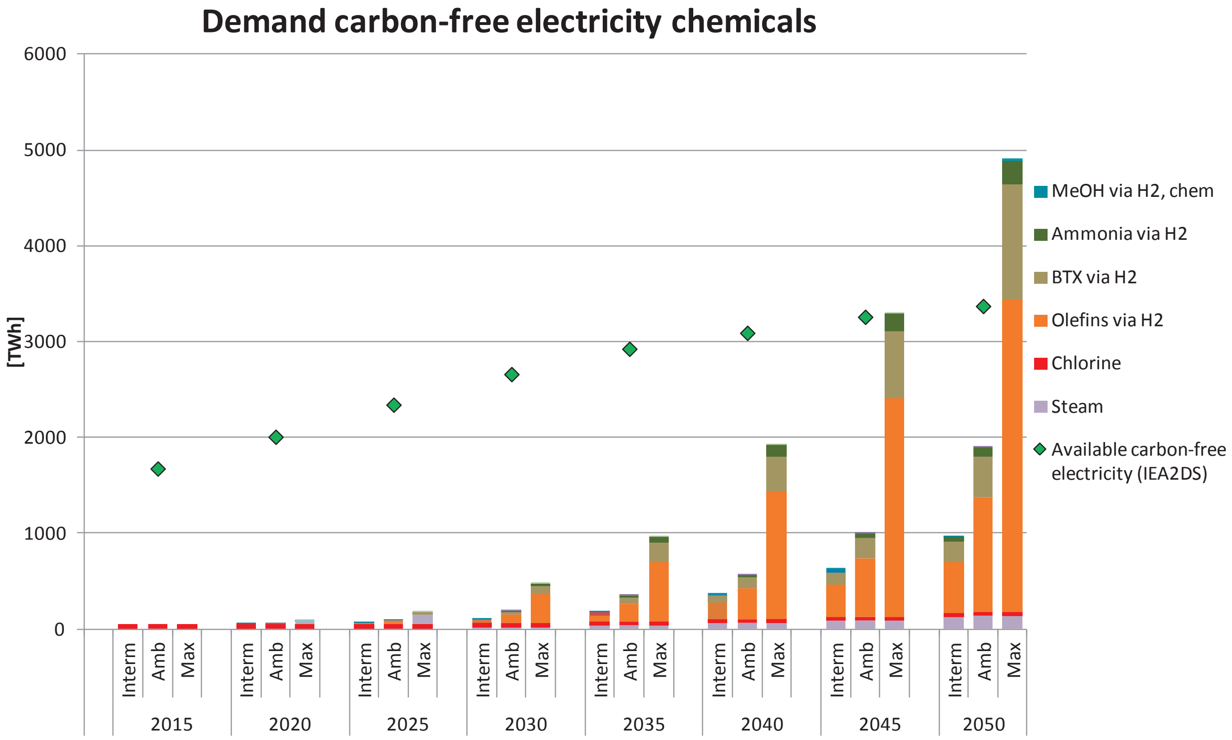
10 Energy and feedstock demand of the different scenarios

10.1 Demand for carbon free electricity

The technologies described in chapter 4 require high amounts of low-carbon electricity. In accordance with several available life cycle assessment studies on renewable hydrogen and chemicals production, this study concludes, that the implementation of electricity-based production does not achieve a positive CO_2 impact, if the current European electricity mix is used. The use of low-carbon free electricity is a prerequisite! It is therefore essential to compare if and how the ambitions of the three scenarios match with the projected availability of low-carbon electricity.

Figure 26 depicts the combined demand for carbon free electricity for the different hydrogen-based technologies both for chemicals only and for chemicals and fuels. Biomass routes have therefore not been included in these charts. The green spots indicate the projected availability of low-carbon electricity, according to the IEA EP2015 2°C scenario. From the model, gross electricity generation from renewable sources (wind, PV, CSP, hydro, geothermal, biomass and waste) as well as nuclear power has been used.

a)



b)

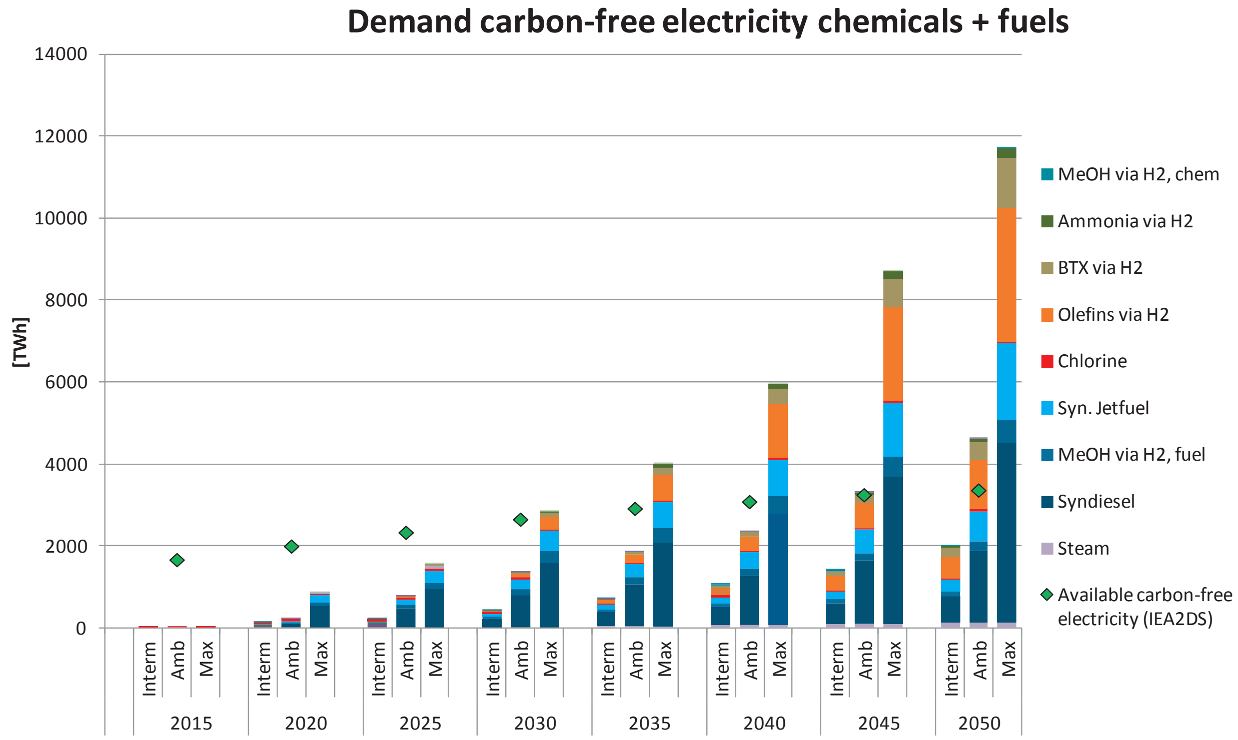


Figure 26: Carbon free electricity demand of hydrogen-based routes in all scenarios; a) chemicals only; b) chemicals and fuels The green points indicate the available carbon free electricity in Europe taken from the IEA ETP energy 2°C model;

The results can be summarized as follows:

- The max scenario would already request all available low-carbon power in 2045 just for chemicals production; in 2050 electricity demand would be at 4900 TWh, which is 140% of the anticipated low-carbon power supply. If fuels are included, demand increases to 11700 TWh, or 350 % of the projected available supply.
- The Amb scenario would consume 1900 TWh for chemical production in 2050, 56% of the anticipated available supply. Including fuels, the demand would be at 4600 TWh, exceeding the available low-carbon power by 37%.
- The least ambitious Interm scenario would still demand 960 TWh (29%) excluding and 2000 TWh (59%) including fuels. It has to be pointed out again, that the Interm scenario only leverages 54% decrease of the CO_2 emissions of the chemical industry expected in 2050, based on chemical production only.

It is obvious that the availability of low-carbon power will be a major critical bottleneck in the deployment of hydrogen based chemical production technologies. This is even more serious, as the IEA 2°C scenario used for these calculations already includes a relatively strong capacity extension of renewable power generation. As a consequence, carbon-neutrality of the

chemical sector very much relies on a much more ambitious extension of low-carbon power capacities, at least a factor 2 of the level anticipated by the IEA. The chemical sector then would demand the output of this additional 100% capacity extension.
It has to be emphasized though, that a large share of the high energy demand of the electricity-based low-carbon pathways can be attributed to the fact, that the target products are built-up from just water and CO_2, thereby not making profit of the high energy content of feedstock that is used in the alternative fossil processes. Energy consumption should therefore be discussed on the basis of the total energy demand, i.e., in case of the fossil processes, including the energy content of the feedstock built-in the target product. Table 34 provides a comparison of the fossil vs. low-carbon routes. The energy gap between the low-carbon compared to the fossil process is lowest for methanol, which is directly built from hydrogen and CO_2. The subsequent products, olefins and BTX, need a second synthesis step, in which 2.3 or 4.3 t methanol respectively are needed as precursors per ton of olefin or BTX.

Generally, many of the described low-carbon processes are not energy efficient, but only have a lower carbon footprint in the defined system. This also means that the carbon-free energy could have a larger effect in other systems. However, it is out of the scope of this study to provide a merit order of different use options for low-carbon electricity in terms of the most (cost) effective emission savings.

Table 34: Total energy demand of fossil vs. electricity-based low-carbon processes

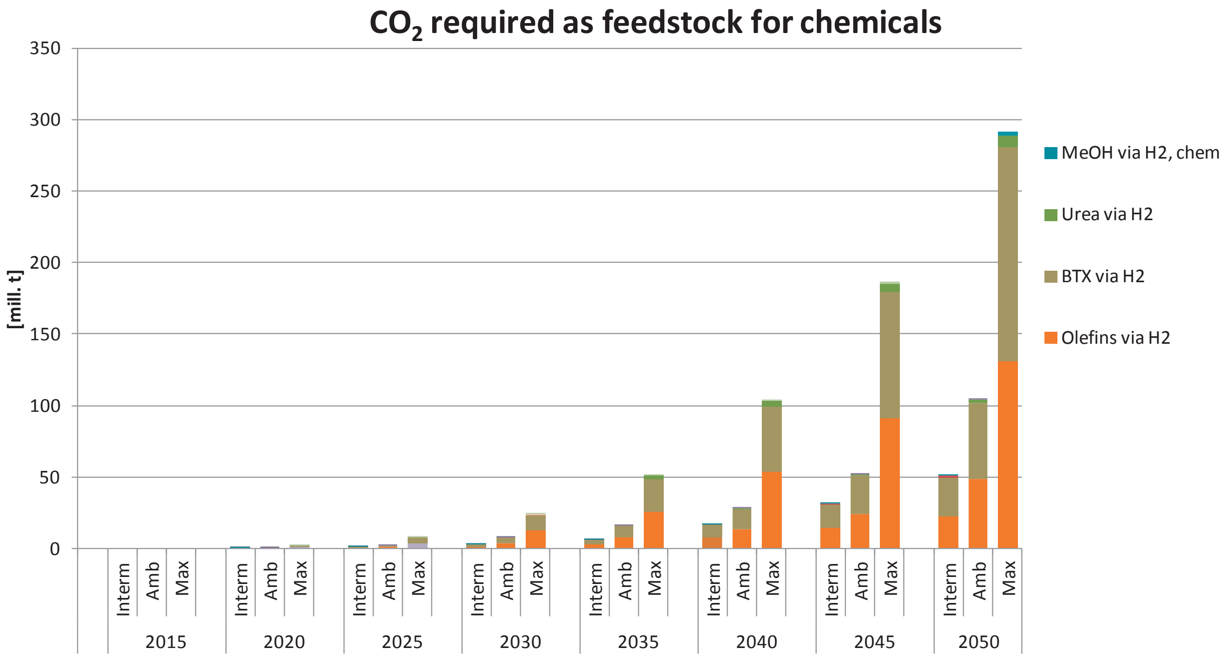
Total energy demand [GJ]	Fossil incl. feedstock	Low carbon via hydrogen and CO_2
Methanol	37.5	41.7
Ethylene	63.6	95.5
Propylene	62.3	95.5
BTX	48	176

As outlined in chapter 8, recycling of polymer waste as feedstock could reduce the demand for de novo synthesis of polymers and subsequently synthesis of monomers and precursors. Moreover, energy recovery from polymer waste can be used to supply part of the process energy. Hence, recycling of polymer waste can impact the overall production volumes and energy requirements decribed in the scenarios. Calculations based on the Accenture study suggest potential energy savings around 57Mtoe or 663 TWh. Comparison with the numbers stated above though turns out to only leverage a small relief of this principal bottleneck.

10.2 Demand for CO_2 as feedstock

Figure 27 depicts the demand for CO_2 as carbon source in the three scenarios. CO_2 demand per unit of production for the different processes has been quantified in chapter 4. The available CO_2 from large sources has been described in chapter 4.10.

a)



b)

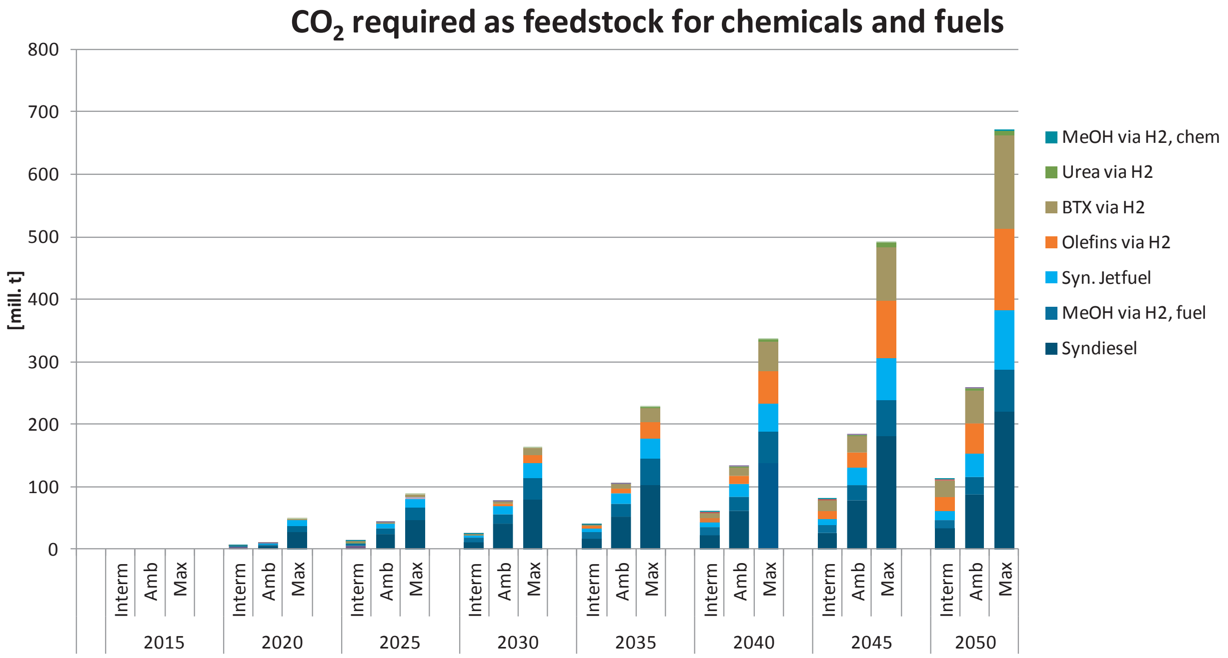


Figure 27: CO_2 as feedstock demand of hydrogen-based routes in all scenarios; a) chemicals; b) chemicals and fuels

CO_2 demand in Figure 27 is always allocated to the final target product. For instance, olefin production does include the CO_2 demand of the intermediate methanol, which is initially produced to supply the MTO process.
It was already concluded in chapter 4.10 that the available CO_2 of 381 Mt in 2050 would be sufficient to supply the demand of chemical production and fuel production in the scenario. This scenario would only require 258 Mt CO_2 in 2050, including fuel production.

The maximum demand for CO_2 as feedstock (max scenario) however would exceed the available sources already in 2045 if fuels are included. In 2050, 673 Mt CO_2 for chemicals and fuels would be required as theoretical upper demand.

10.3 Biomass as feedstock demand

The processes discussed in chapter 6 rely on biomass as a feedstock. Biomass demand per unit of production has been discussed there. For the scenario work bioethanol production from sucrose, starchy and lignocellulosic feedstocks, methanol production via gasification of lignocellulosic and waste biomass, and olefin production following bioethanol from wood production have been included.
For the calculation of bioethanol as fuel it is assumed that 100% of the feedstock is sucrose/starch biomass at present (sugar beet as reference) and that lignocellulosic biomass will increase to a share of 25 % by 2050 (wood as reference).
Figure 28 shows the aggregated biomass demand for the three processes in all scenarios. About 250 Mt biomass would be demanded in the max scenario. It has to be emphasized here, that the max scenario does not anticipate a 100% bio-based production. Nevertheless 250 Mt biomass correspond to 110 Mtoe, which would roughly correspond to 30% of the available biomass for non-food and feed applications. Biomass availability has been discussed in chapter 6.7.

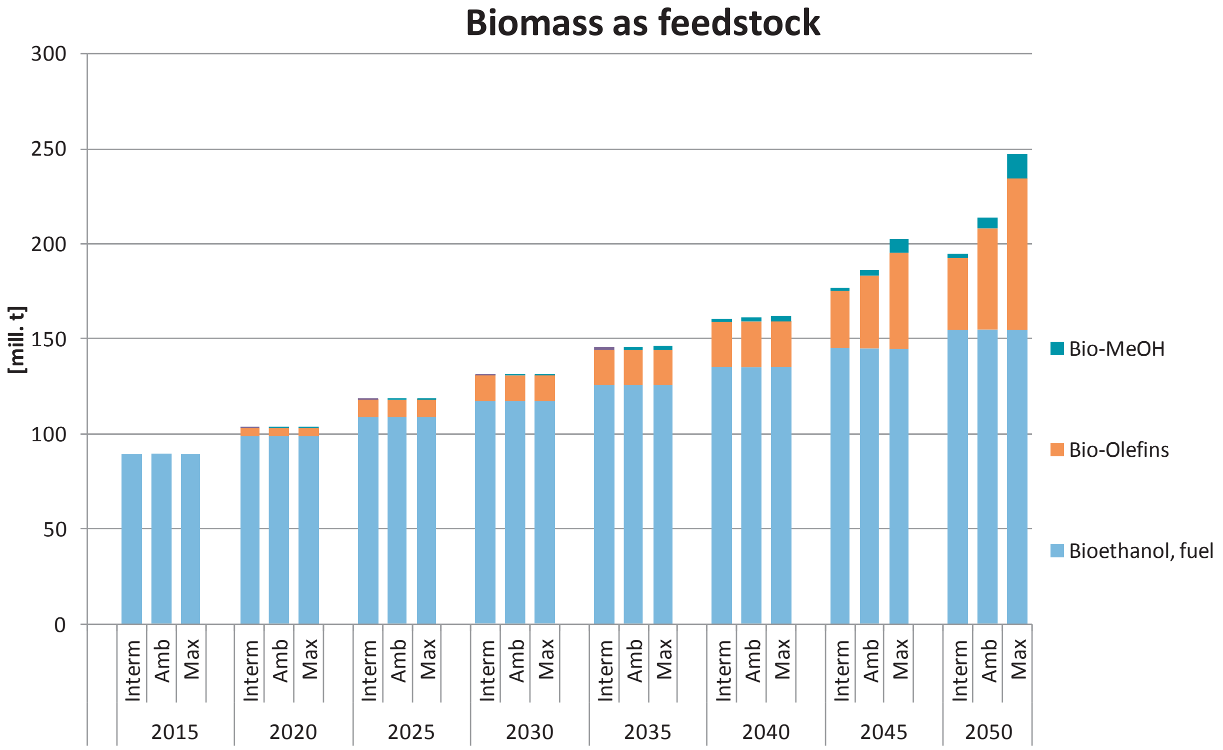


Figure 28: Biomass demand as feedstock for all scenarios

11 Economic implications of the scenarios

The transformation of the main processes of the chemical industry will require substantial investment into new processes with their respective process plants and equipment. Europe's chemical industry is quite a mature industry and many existing plants have long outlived their technical lifetime. Thanks to constant investments, aiming to increase process and plant efficiencies, Europe's chemical industry, notwithstanding its high average plant lifetime, is still outperforming most other world regions on energy efficiency. However, most new large projects are commissioned elsewhere and these regions, implementing the most recent technologies, are quickly catching up.

Even if Europe's chemical industry could defend its leadership position in energy efficiency in the long run, this would clearly not be enough to facilitate the transformation into a low-carbon industry. On the other hand, technology options to impact the chemical industry's CO_2-footprint will not come for free, both in new investments and in reducing fossil fuel based production capacities. This has been extensively discussed in previous chapters.

Within the scope of the study, the relative extend of the transformation of the main processes has been approximated. These calculations are based on a set of assumptions outlined below.

The main driver to improve plant performance is to build new production capacity or to retrofit existing production capacity with state-of-the-art technology. The required investment is depreciated over 10 years with an interest rate of 10%. With the notable exception of chlorine production plants, all existing plant capacity is assumed to be depreciated at the starting point of the calculation (2015). Chlorine production is currently undergoing substantial investments for the decommissioning of mercury-process based plants; most of them are replaced by membrane-based processes (see chapter 3.3). For chlorine, half of the production capacity is therefore considered to be only 5 years old.

All costs and prices are expressed as nominal values (2015) and are not discounted. The development of fossil fuel prices is taken from IEA ETP 2016 [[128]]. Electricity prices are assumed to remain constant at 40 €/MWh. For water electrolysis a linear decrease in investment cost from 1450 to 375 €/kW from 2015 to 2050 is explicitly taken into account. The investment costs for all other technologies are considered to be constant over the range of this study. Overall production of a given product increases by 1% p.a. The price for CO_2-emission certificates is expected to rise by 10% each year from the current level of 7 €/tCO_2 up to 196 €/CO_2 in 2050.

Table 35 summarizes the assumptions and the calculated specific production costs for 2015 for conventional production.

Table 35: Economic parameters for the different processes under consideration.

Product	Conventional Process	CAPEX conventional €/tproduct	OPEX conventional (without energy and feed) €/tproduct	Low-carbon process	CAPEX low-carbon €/tproduct	OPEX low carbon (without energy, feed, CO_2) €/$t_{product}$	Specific production cost (including energy, feed, CO_2) €/$t_{product}$
Chlorine (including H_2, NaOH)	Membrane electrolysis	1000	150	n/a			
Ammonia	Steam reforming, ammonia synthesis	670	100	H_2O electrolysis, ASU, ammonia synthesis	1450	290	427
Methanol	Steam reforming, methanol synthesis	400	60	H_2O electrolysis, CO_2-capture, methanol synthesis	1450	290	473

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[128] http://www.iea.org/etp/etp2016/

Ethylene	Steam cracking	1200	180	MTO	300	45	1082
Propylene	Steam cracking	1200	180	MTO	300	45	1063
BTX	Steam cracking	1200	180	MTA	300	45	956

11.1 Production Costs

Overall production costs are calculated as sum of conventional (con) production costs and low-carbon technology (ren) costs. Within the different scenarios, the relative development of conventional and low-carbon technology differs and hence the relative investments into these technologies. All together, these products sum up to current overall production cost of nearly 50 bn € p.a. in 2015 which increases to 103 bn € within the BAU scenario in 2050 due to increased production and higher CO_2-prices. Figure 29 compares the total production costs for the different scenarios.

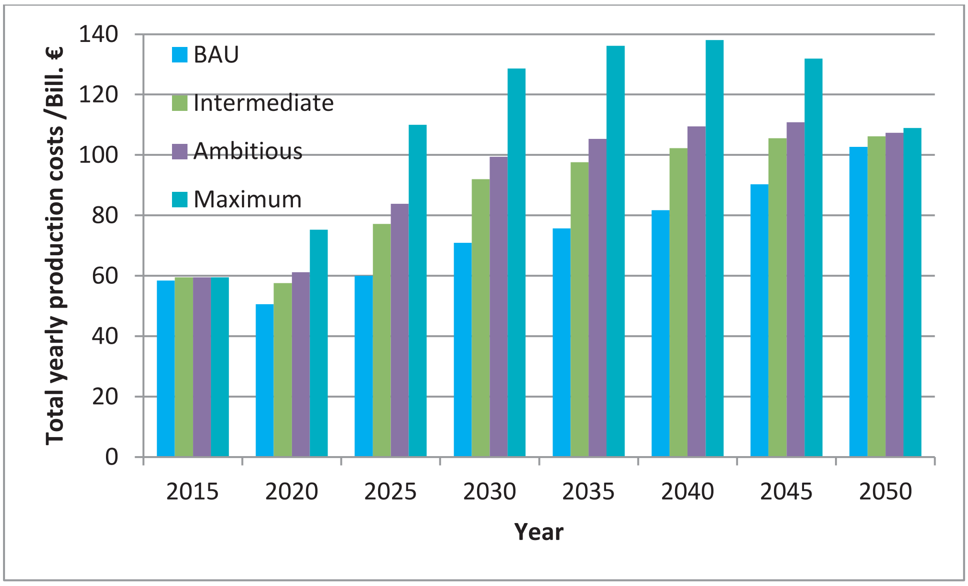

Figure 29: Development of total yearly production costs within the different scenarios.

All scenarios lead to a significant increase of total production costs compared to the BAU scenario. The impact of efficiency improvement technologies is part of all scenarios except BAU.

The strongest increase is shown within the Maximum scenario due to a complete replacement of conventional plants by low-carbon technologies. The drop of total production cost in 2045 and 2050 for the maximum scenario is caused by significant compensation for CCU via CO_2-emission certificates. The following tables (Table 36 - Table 38) summarize the cumulative investment (retrofitting existing plant and building new capacity) until 2050 for the different products under consideration.

Table 36: Total investment costs (retrofitting and new capacity) for the different products within the different scenarios. The effect of implementing efficiency measures on BAU is also included (Efficiency).

Mill. €	Chlorine	Ammonia	Urea	Methanol	Ethylene	Propylene	BTX	Sum	Yearly average
BAU	6087	9172	4267	435	20871	16385	15070	72287	2065
Efficiency	29943	64954	24013	3384	147814	116041	106730	492879	14082
Intermediate	29943	67902	25286	178322	116882	91758	84395	594488	16985
Ambitious	29943	73593	27093	260089	112073	87983	80923	671697	19191
Maximum	29943	76611	32906	570699	89421	70200	64567	934347	26696

Table 37: Investment costs (retrofitting and new capacity) for conventional production technologies of the different products within the different scenarios. The effect of implementing efficiency measures on BAU is also included (Efficiency).

Mill. €	Chlorine	Ammonia	Urea	Methanol	Ethylene	Propylene	BTX	Sum	Yearly average
BAU	6087	9172	4267	435	20871	16385	15070	72287	2065
Efficiency	29903	64954	24013	3384	147814	116041	106730	492839	14081
Intermediate	29903	45687	14999	2590	103968	81620	75071	353839	10110
Ambitious	29903	41052	13463	2359	93420	73339	67454	320990	9171
Maximum	29903	4254	6948	1374	49604	38941	35817	166841	4767

Table 38: Investment costs (retrofitting and new capacity) for the low-carbon production technologies of the different products within the different scenarios. The effect of implementing efficiency measures on BAU is also included (Efficiency).

Mio. €	Chlorine	Ammonia	Urea	Methanol	Ethylene	Propylene	BTX	Sum	Yearly average
BAU	0	0	0	0	0	0	0	0	0
Efficiency	40	0	0	0	0	0	0	40	1
Intermediate	40	22215	10287	175732	12913	10138	9324	240649	6876
Ambitious	40	32542	13630	257730	18653	14644	13469	350708	10020
Maximum	40	72357	25958	569325	39817	31259	28751	767506	21929

The deployment of low-carbon production technologies as described in the different scenarios requires massive investments in new plants. Comparing the impact for the different scenarios shows a total yearly investment of 26.7 bill. € within the Max scenario, with 4.8 billion € for conventional technologies and 22 bill. € for low-carbon technologies. For the Amb. scenario the toral yearly investment amounts to 19.2 bill. € with 9.2 bill. € total yearly investment into conventional technologies and 10 bill. € of total yearly investment into low-carbon technologies. The respective numbers for the Inter.-scenario are 16.9 total yearly investment, split into 10.1 bill. € for conventional technology and 6.9 bill. € for low-carbon technology. Efficiency measures are applied to both, conventional and low-carbon technologies within all scenarios except BAU.

11.2 Total production costs and CO_2 avoidance costs for individual chemical products

The following subchapters provide a more specific economic analysis for the individual products. Within each scenario, the production costs for conventional, fossil-based technologies (indicated as “con” in the graphs) and the low-carbon technology (indicated as renewable “ren” in the graphs) develop independently as a function of their respective energy costs, CO_2 cost, technology development and their deployment. They are therefore depicted separately to identify the break-even points when both technologies within the respective scenario provide the product at the same costs within the assumptions of the model.

CO_2 avoidance costs per unit product (ton of product) within a scenario are calculated as difference of unit production costs (PC) without the costs or compensation of CO_2-certificates divided by the difference of total CO_2 emissions versus the BAU scenario.

$$C(CO_{2,avoid.}) = \frac{\left[\sum_{con,ren} PC(scenario) - PC(BAU)\right]}{\left[CO_2(BAU) - \sum_{con,ren} CO_2(scenario)\right]}$$

For all products, the low-carbon technologies cause higher production costs per unit than the conventional technologies. Therefore, negative CO_2 avoidance costs can only occur in case of larger emissions from the low-carbon technologies compared to the respective conventional production. Such larger emissions are caused, when the electricity required by the hydrogen based low-carbon technologies is supplied as grid power based on the current European average electricity mix. From a climate perspective, it would not be desirable to implement the process under these circumstances. Negative CO_2 avoidance costs are therefore not depicted in the graphs in the following sections. It is therefore a necessary requirement to have the power sector sufficiently decarbonised before electricity-based low-carbon technologies can make a positive impact on the reduction of GHG emissions. Prior to the necessary decarbonisation of power, the chemical industry would need to make sure that only low-carbon electricity is used, e.g. by using electricity from own wind energy parks instead of grid electricity.

11.2.1 Ammonia

Figure 30, depicts the calculated total production costs for ammonia within the different scenarios.

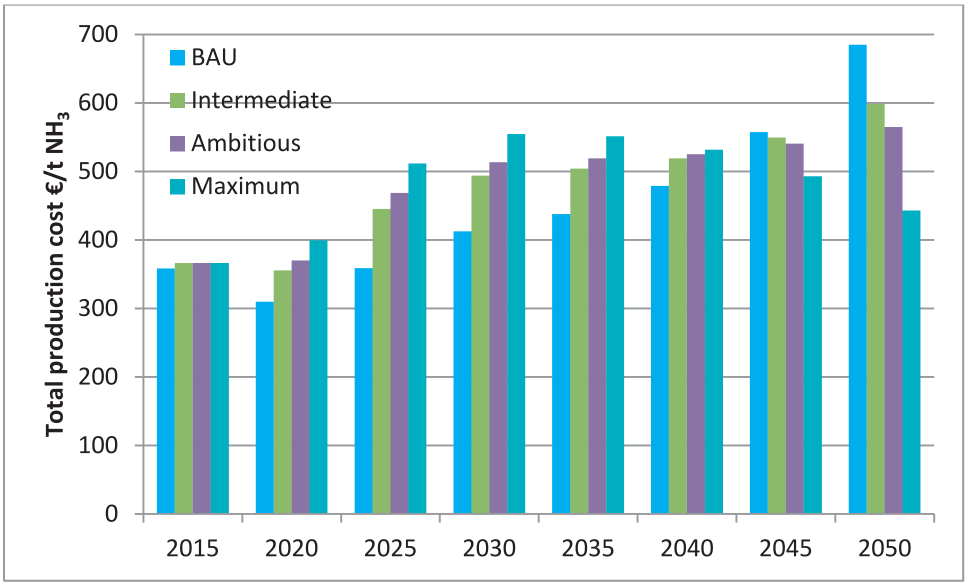

Figure 30: Development of total production costs of ammonia within the different scenarios.

Conventional ammonia production cost is dominated by fuel and feed cost. Implementing efficiency measures leads to slightly higher production costs than in the BAU scenario. The rise of cost is only partially due to new capacity, but dominated by an increase in the cost of CO_2-certificates, which amount to half of the total production cost in 2050 within the BAU scenario. The Intermediate, Ambitious and Maximum scenarios deploy low-carbon technologies, which initially leads to higher total production costs for these scenarios. As a significant drop in cost for electrolysers is assumed, the deployment of low-carbon technologies becomes cheaper and the low-carbon ammonia total productions costs are eventually dominated by the cost of electricity. Conventional ammonia production costs increase over time by the assumed rising costs for CO_2 certicates. The total production costs for ammonia via conventional and low-carbon processes within the various scenarios are displayed in Figure 31. Initially, low-carbon production processes produce at significantly higher cost than conventional processes but benefit in the long run by the decay of electrolyser costs and the rise of CO_2-certificate prices until 2050.

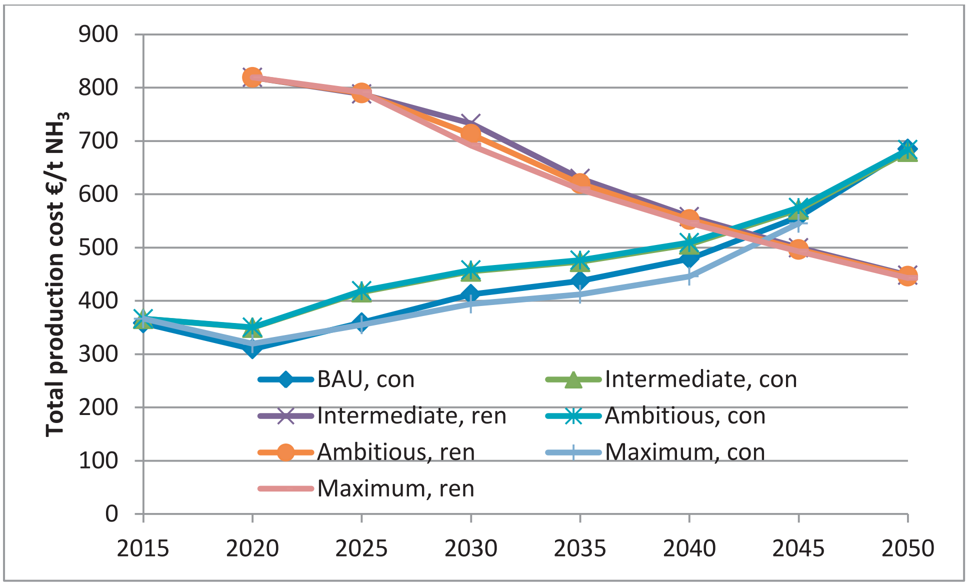

Figure 31: Total production costs of NH_3 by conventional (con) and low-carbon (ren) processes within the different scenarios, including costs for CO_2-certificates.

CO_2-avoidance costs are as the difference in cost over calculated with respect to the BAU scenario, i.e. conventional technology without the implementation of efficiency measures. Low-carbon ammonia is produced by water electrolysis, air separation and the actual ammonia synthesis. The amount of CO_2 emissions associated with low-carbon ammonia production depends on emissions caused by the generation of electricity. Within the projected development of CO_2 emissions of grid electricity, implementation of low-carbon ammonia production will only lead to a net reduction of CO_2 emissions from 2025 to 2030 onwards, once grid electricity is sufficiently decarbonized, compare Figure 32: However, in the long run the scenarios suggest CO_2 avoidance costs in the order between 60 (Maximum) and 200 €/t CO_2 avoided.

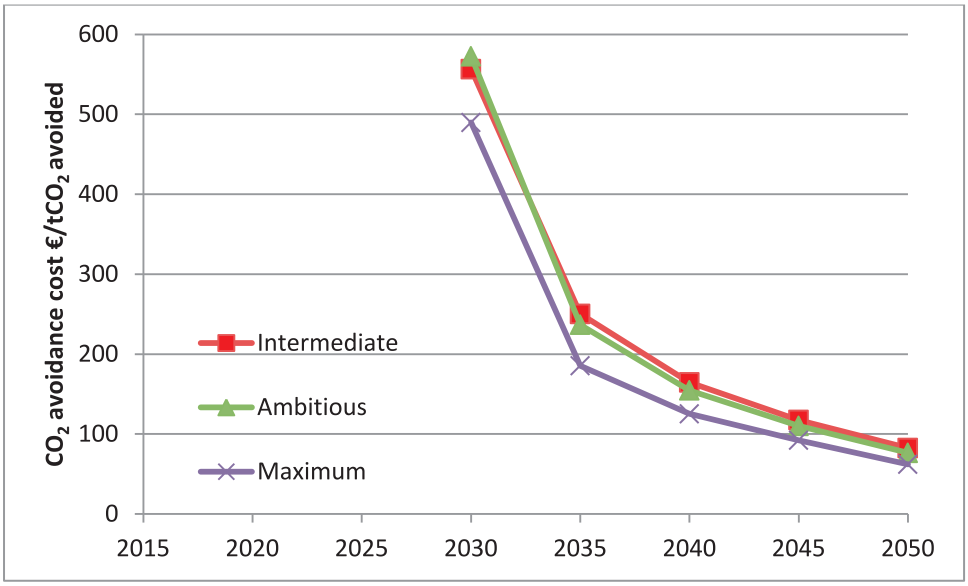

Figure 32: CO_2 avoidance costs for the production of ammonia. . Before 2030 the low-carbon production of ammonia emits more CO_2 than the conventional process due to carbon-intensive power generation.

11.2.2 Chlorine production

Figure 33 depicts the calculated production cost for chlorine production within the different scenarios.

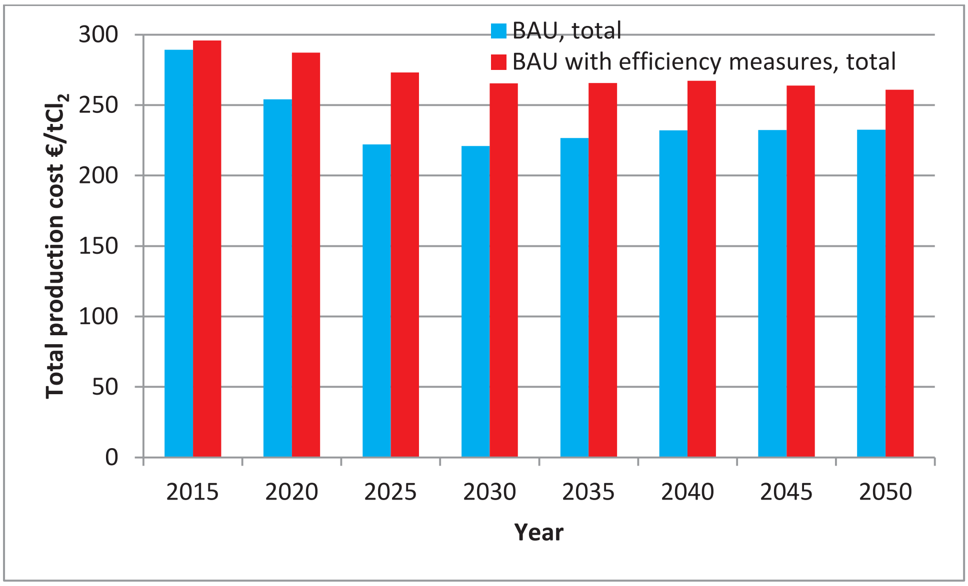

Figure 33: Chlorine production costs in the BAU with and without efficiency masures

Within the modeling, conventional chlorine production does not have a low-carbon process related to it. While there are different processes operational and new technology, like oxygen depletion electrodes can be deployed to significantly reduce energy requirements for chlorine production, the site specific configuration depends strongly on the respective downstream processes to accommodate the hydrogen byproduct and to purify the caustic soda byproduct to market specifications. The model associates all costs for the chlorine production to the chlorine product, with no costs being attributed to the byproducts hydrogen and caustic soda. Therefore, as far as the modeling is concerned, there are no scenarios implementing an alternative low-carbon technology option. However, the implementation of efficiency measures can have an effect. Chlorine production is already subject to significant investment into new plants or retrofitting existing plants due to industry`s commitment to phase out the mercury-based processes by the end of 2017, leading to a significant modernization of the existing plant portfolio. Additional efficiency measures are therefore relatively less effective.

Chlorine production becomes a low-carbon technology via the changing of CO_2 emissions of the electricity generation used. Efficiency measures and developing technology reduce the amount of electricity required, thereby lowering the CO_2 emissions associated with chlorine production. While these emissions are generally allocated to the power sector and not to the chemical industry, they have been included in this report, since the chemical industry claims ownership of the process and attempts to lower its impact on greenhouse-gas emissions. However, CO_2-avoidance costs, Figure 34, by efficiency measures to the chlorine production processes are relatively expensive and becoming more expensive in the future due to the rapid reduction of the CO_2 emissions of grid electricity. There might be a number of good reasons to implement and deploy technological improvements and efficiency measures into existing processes, its impact on CO_2-reduction will however be not be cost-effective compared to the reduction of emissions within the power sector.

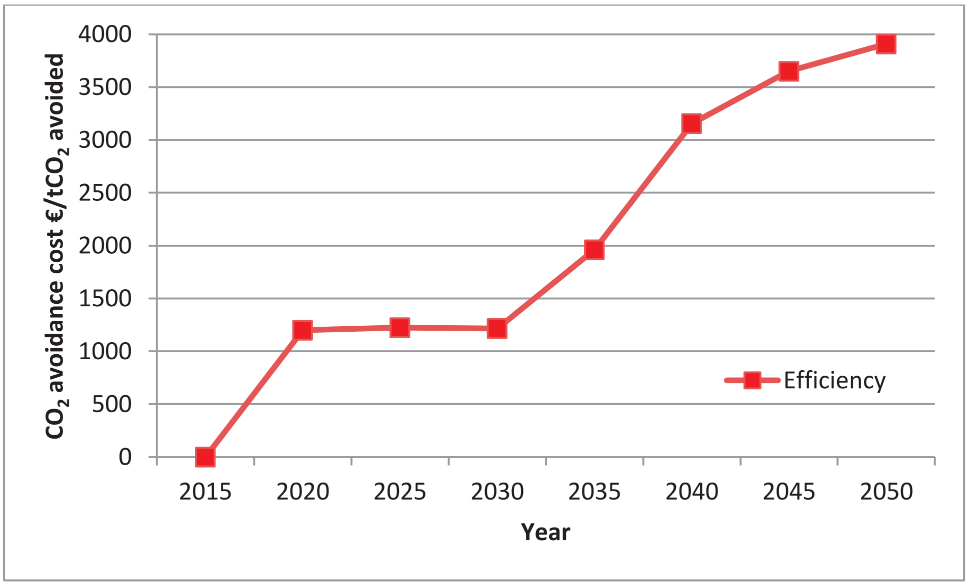

Figure 34: CO_2 avoidance costs for efficiency measures in chlorine production

11.1.3 Urea

Urea is a downstream product of ammonia and, generally produced within integrated plants with ammonia production. It is the largest carbon-capture and utilisation (CCU) process currently in existence. Its cost development is therefore especially sensitive to changes in prices and allocation rules of CO_2 emission certificates. Within the scope of this modeling approach, it is assumed that urea production cost benefit from being a sink for CO_2, which goes beyond the current policy within Europe's emission trading system[129].

Urea production is closely linked to ammonia production, both within the conventional and the low-carbon process schemes. Within the conventional process route, CO_2 produced by steam reforming is separated from the hydrogen to allow the production of ammonia. Therefore, no additional cost for CO_2-separation is allocated to urea in the conventional process route. . However, urea production as a down-stream process of low-carbon ammonia requires an external CO_2-source. The additional energy requirement for CO_2 capture as feedstock for low-carbon urea production needs to be taken into account. It also leads to some additional greenhouse gas emissions. However, within the model, CO_2 is made available to the urea production process without additional cost associated to its separation or purification.

Figure 35 depicts the development of total urea production costs within the different scenarios. All scenarios that include a significant contribution by low-carbon technologies (Intermediate, Ambitious, Maximum) benefit in the long run from the relative lower production cost for low-carbon ammonia caused by reduction of cost of the electrolyser.

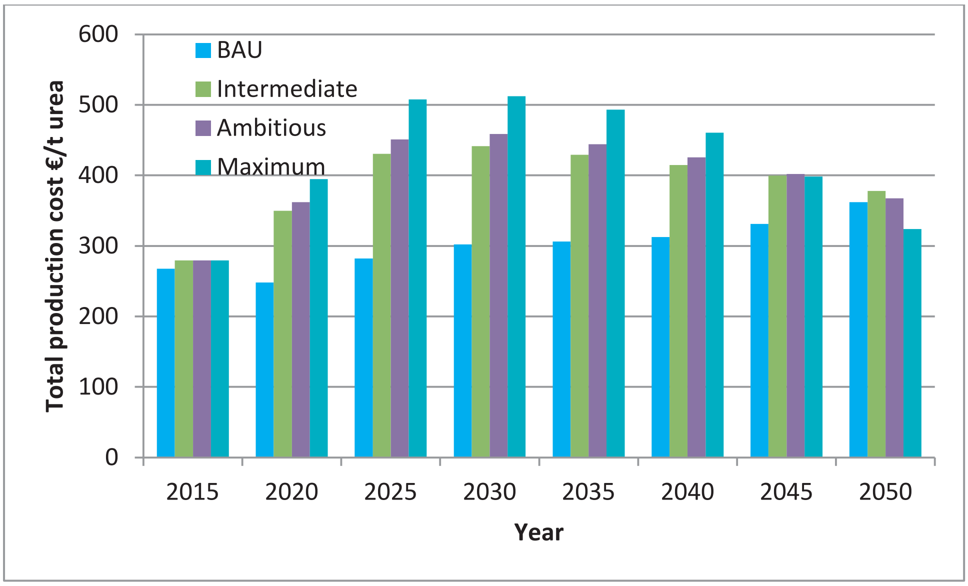

Figure 35: Total costs of urea production within the different scenarios.

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[129] Under current rules, CCU is not supported by the European Emissions Trading System, since it (with a few notable exceptions) does not lead to a permanent removal of CO_2 from the atmosphere.

Both, conventional and low-carbon urea production processes are dominated by the cost for the ammonia feed. Both processes do benefit by increased compensation for CCU, as displayed in the following Figure 36 and Figure 37. However, the effect only becomes significant from 2040 onwards, where costs for CO_2-certificates are expected to rise beyond 75 €/t CO_2.

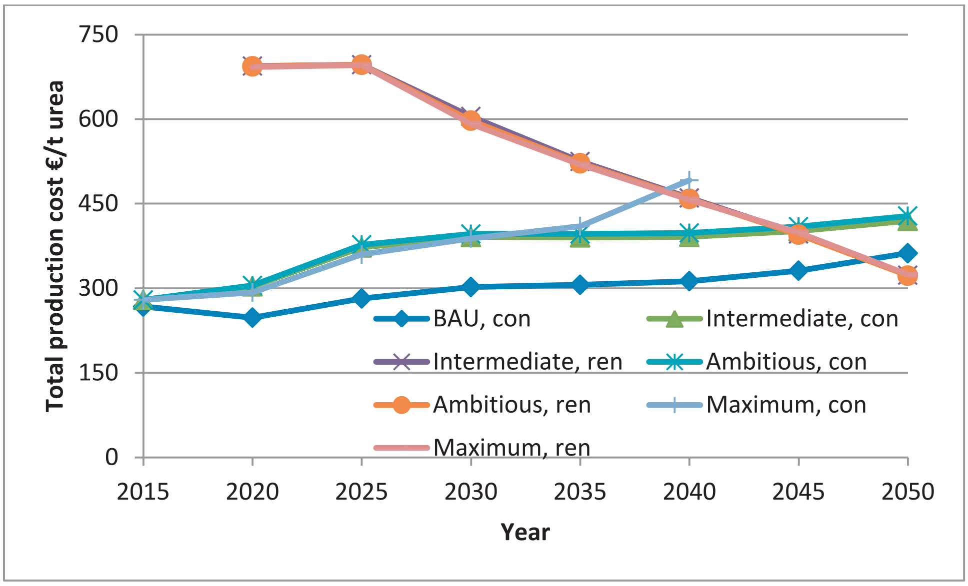

Figure 36: Development of total production costs of urea with compensation for CO_2 utilisation; Conventional (con) and low-carbon (ren) production is indicated for the various scenarios.

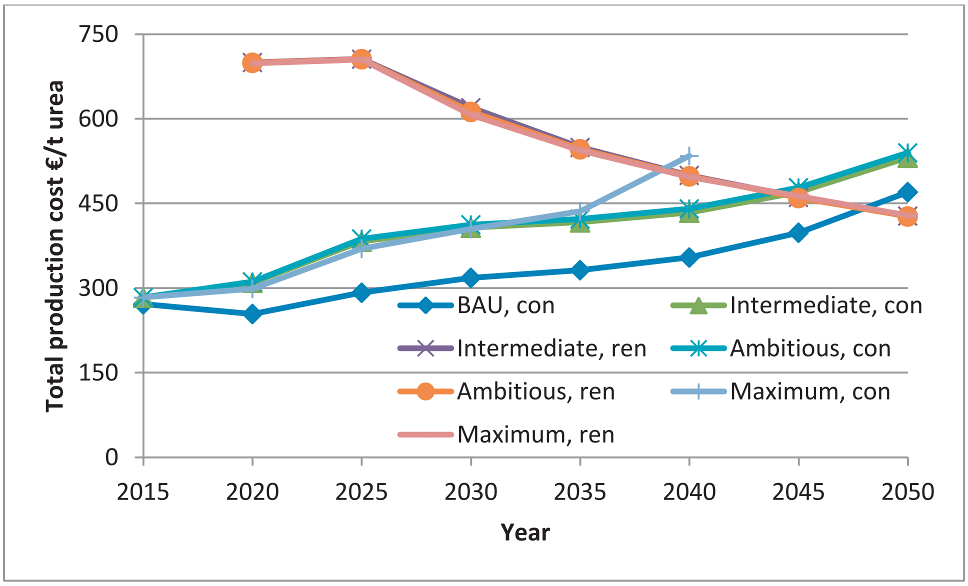

Figure 37: Development of total production cost of urea without compensation for CO_2 utilisation; Conventional (con) and low-carbon (ren) production is indicated for the various scenarios.

Both, the conventional and low-carbon process are net sinks for CO_2, due to the reaction to form urea consumes CO_2 in the ratio of 44/60. To that extend, the CO_2-avoidance costs for urea production are given by its total production cost multiplied by 60/44. In comparison to this sink, any improvements on the process itself are marginal and much more expensive.

11.1.4 Methanol

Methanol takes a central role in all scenarios, since its low-carbon route is the foundation to substitute conventional products of steam cracking. Besides the currently low overall conventional production in Europe, low-carbon methanol production needs to expand rapidly in order to substitute significant parts of current conventional cracker products. As with urea, low-carbon methanol production is a net sink for CO_2 and the overall cost benefit from compensation with CO_2 emission certificates. CO_2 required for low-carbon methanol production is taken into account, both energetically and with respect their GHG emissions, but the CO_2 capture is not associated with any cost. Additionally, as in the case of low-carbon ammonia production, development of methanol production cost also benefit greatly from reduced costs for electrolyzers as the time progresses. The total production cost for methanol is displayed in Figure 38.

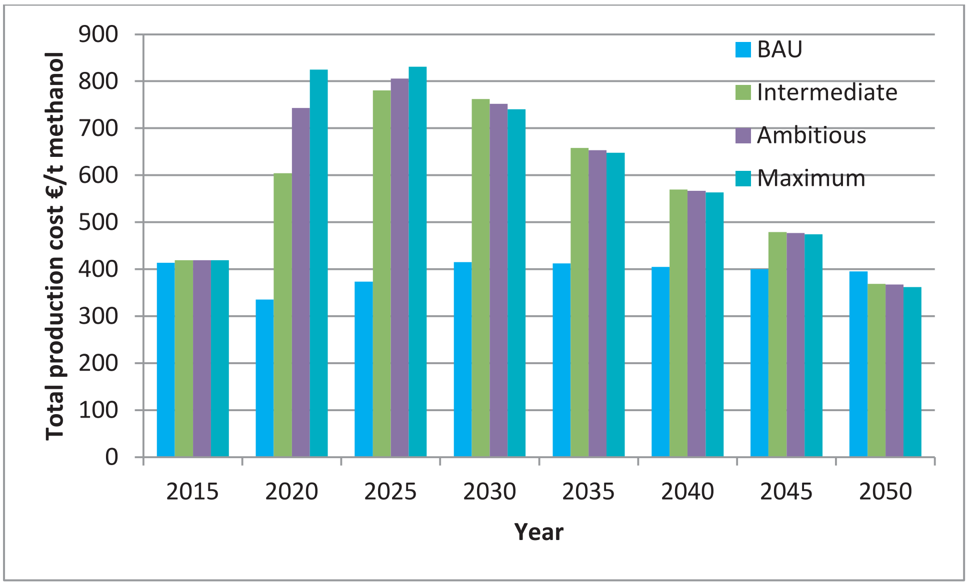

Figure 38: Total production costs for methanol within the different scenarios.

Conventional methanol production is dominated by its feed and fuel costs, while the low-carbon methanol production is dominated by electricity cost and investment cost due to the massive expansion of plant capacity within the timeframe investigated in this study.

Figure 39 shows the total production costs for methanol for conventional and low-carbon production within the different scenarios, including and excluding respectively the costs for CO_2

certificates for the conventional processes and compensation for CO_2 for the low-carbon technologies.

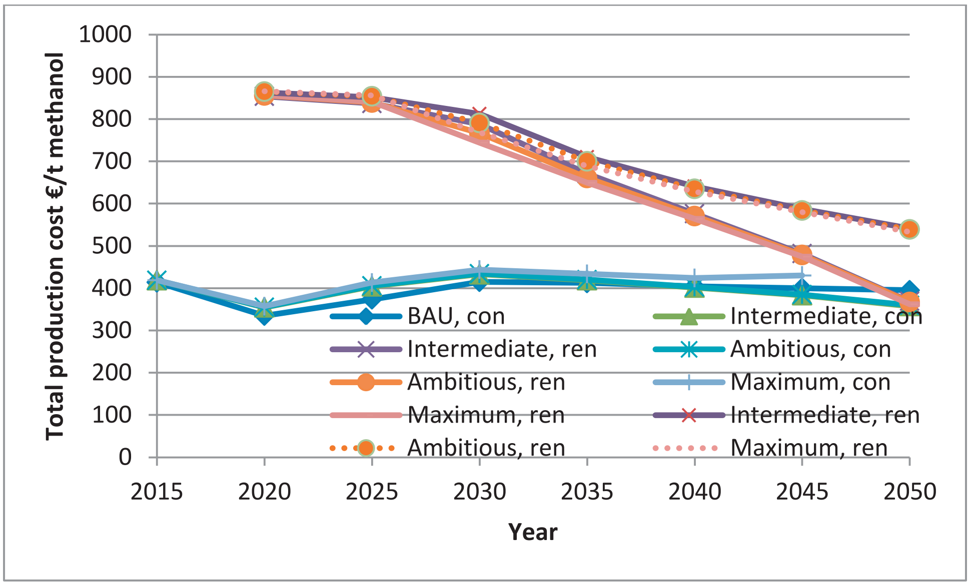

Figure 39: Total production costs for methanol for conventional and low-carbon production within the different scenarios, including certificate costs for CO_2 (conventional, con) and compensation for CO_2 (low-carbon, ren). The set of dotted lines on the top display the respective results without monetary compensation for CO_2 utilization.

With respect to CO_2 avoidance costs, conventional methanol production has a significant component of CO_2 being released by the process itself, the amount depending on the composition of the feed. Additional CO_2 emissions occur due to fuel and electricity used in the process. The latter emissions are subject to incremental process improvements, while the former cannot be avoided. In contrast to the conventional process, the low-carbon process acts as a net sink for CO_2.

As can be seen in Figure 40, the CO_2 footprint of the grid electricity compensates emissions savings and only leads to a net reduction of CO_2 emissions from 2035 onwards. Efficiency measures within the conventional process can lead to reasonable CO_2 avoidance costs within the timeframe of the model.

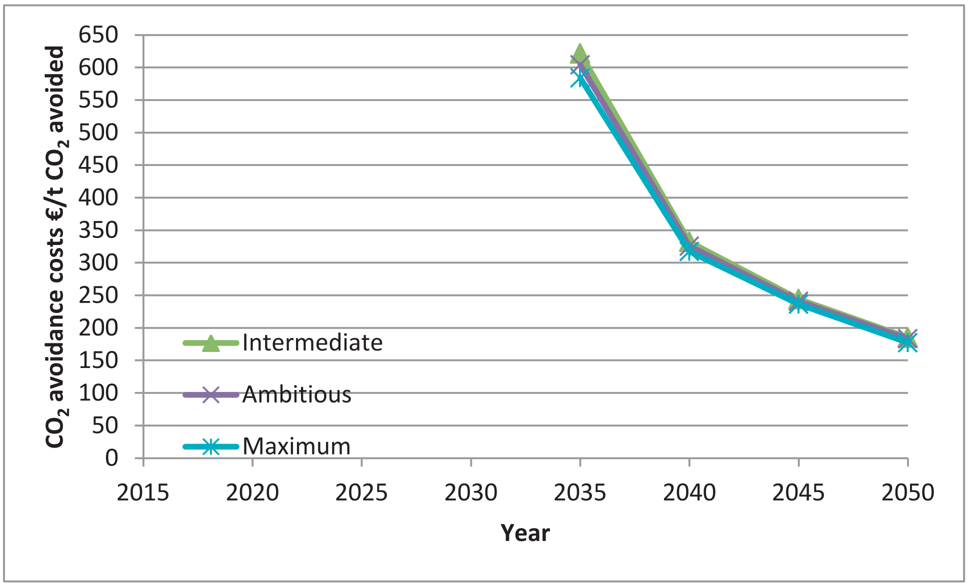

Figure 40: CO_2 avoidance costs for methanol production

11.1.4 Ethylene, propylene and BTX

Cracker products are the starting point of many value chains within the chemical industry. Europe’s crackers are based on naphtha as feedstock and provide a mix of, among others, ethylene and propylene (HVC) and BTX compounds for further transformation. These products will still be required and alternative routes need to be accessed in order to produce them in more sustainable fashion.

Within this study, low-carbon methanol as precursor for Methanol-to-Olefines and Methanol-to-Aromatics processes have been investigated as the predominate routes. The total production cost for olefins and BTX are displayed in Figure 41, and as function of conventional and low-carbon processes in Figure 42. Conventional total production costs are dominated by feed and fuel costs (naphtha), while the low-carbon routes via methanol are dominated by the costs of methanol.

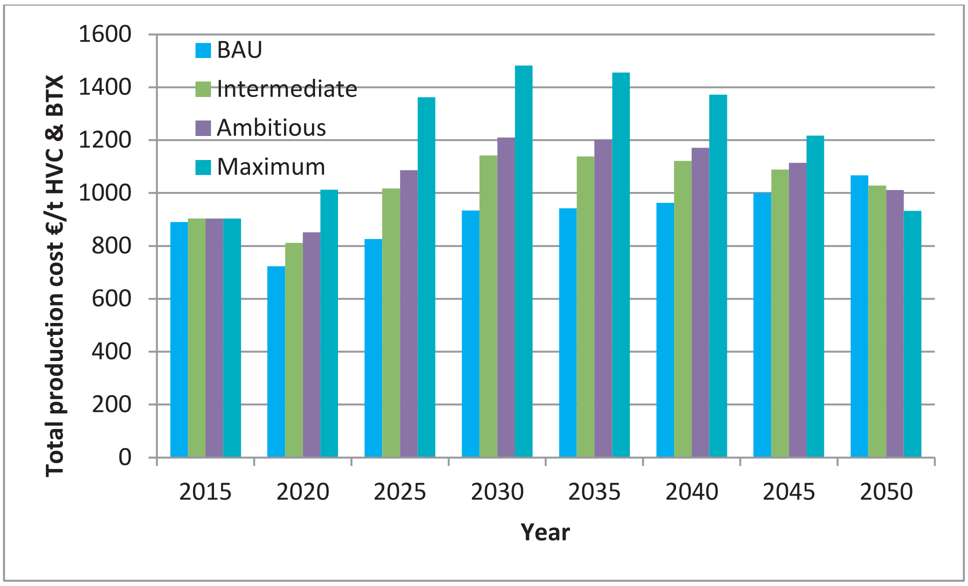

Figure 41: Total production costs for cracker products within the different scenarios

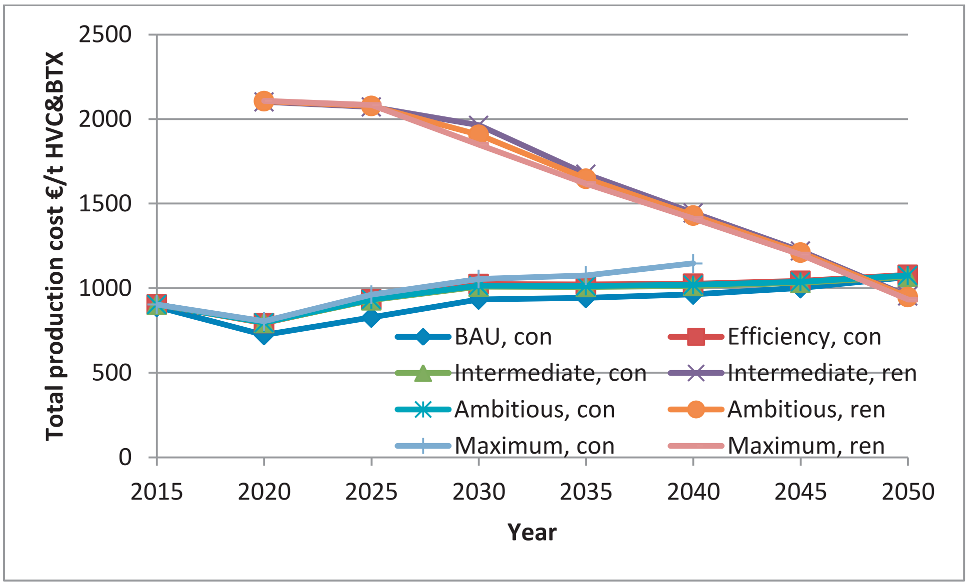

Figure 42: Total production costs for conventional (con) and low-carbon (ren) process routes within the different scenarios

Any compensation for carbon utilization is assigned to the methanol precursor for the MTO and MTA process routes. In combination with highly efficient conventional steam cracking this leads to rather high CO_2-avoidance costs, see Figure 43.

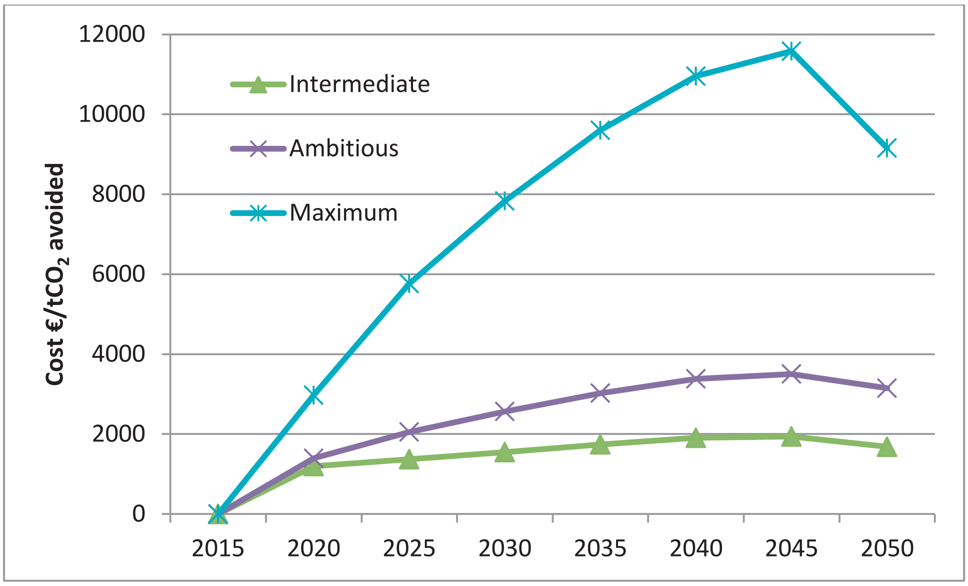

Figure 43: CO_2-avoidance costs for HVC&BTX as a function of the different scenarios.

11.2 Summary and impact of policy measures

The production costs within the BAU scenario are dominated by the development of fossil fuel prices, with ammonia being the notable exception. Ammonia production costs towards 2050 are dominated by prices of CO_2 emission certificates. The Intermediate scenario achieves higher energy efficiency by an increased improvement rate, both in the conventional and renewable technology development that slowly finds its way via retrofitting and new capacity into the plant ensemble. Final production costs for 2050 are lower for chlorine production which benefits most by a significant decarbonisation of the required electric energy for the electrolytic process. Additional investment costs for low-carbon ammonia production are offset by reduced CO_2-emissions, once the CO_2-emission certificate price level is high enough. Low-carbon methanol production in combination with MTO and MTA starts to substitute steam cracking and also benefits from high CO_2-certificate prices by introducing negative emissions. However, as a consequence HVC production on average faces a higher feedstock price compared to a conventional plant ensemble. Within the Ambitious scenario, the final level for specific production costs only reaches BAU levels for methanol and propylene, while all other products have increased specific production costs of 15-45% to accommodate. The Maximum scenario leads to similar costs for all products as the BAU scenario in 2050 if monetary compensation for CO_2 utilization is taken into account.

The dominant feature within the latter scenarios is the large increase in low-carbon methanol production capacities. Methanol specific production costs rise significantly with time due to large investments into new capacity. Only very high price levels for CO_2 emission certificates could eventually offset the burden of the additional investment costs. Under current regulations however, CCU is not considered as negative emissions. The sensitivity of the methanol production costs based on these different policy effects within the different scenarios is depicted in Figure 44.

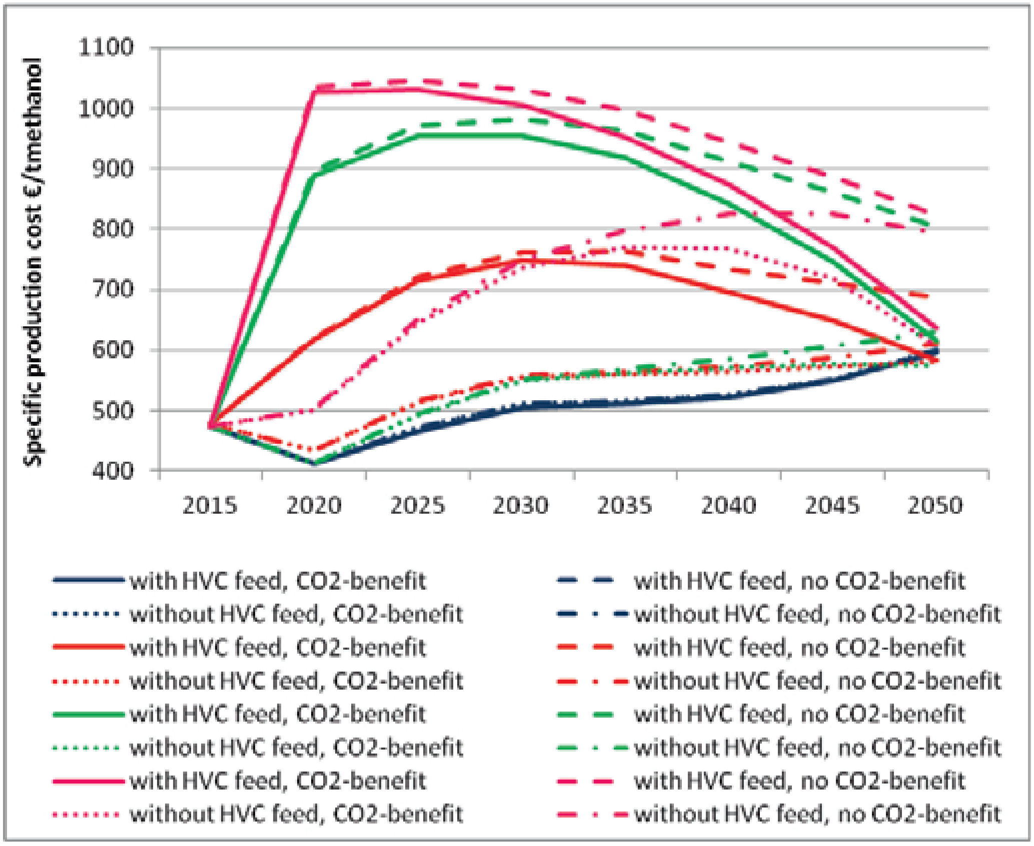

Figure 44: Sensitivity of CO_2 emission allocation on the specific production costs of methanol. "With HVC feed" indicates low-carbon methanol production volumes required for MTO and MTA routes, while lines "without HVC feed" refer to methanol production volumes consistent with current requirements. Blue lines indicate the BAU scenario, red lines indicate the Intermediate scenario, green lines indicate the Ambitious scenario and magenta lines indicate the Maximum scenario.

12 Research, development and innovation requirements

Within this study a large field of technologies has been investigated. This chapter is dedicated to research, development and innovation (RD&I) needs A detailed roadmap from research to commercial deployment for all these technologies is beyond our scope and hence not intended here. A lot of roadmaps and other studies have been cited in this report. Table 39 therefore provides an overview on important and relevant RD&I priorities based on these documents, e.g. references [11], [19], [28] and [130].

Table 39: RD&I topics relevant for a low-carbon chemical sector

Area	Priority	RD&I topic
Power to Heat	Reversible power-to-heat systems	producing heat by an electrically driven heat pump at low electricity prices and to produce electrical power ina reverse mode
	multifunctional equipment to increase flexibility	Alternative use of either natural gas or electricity, depending on the prevailing energy prices, including control strategies
	technologies at higher temperature levels (> 250 °C)	• electrically driven heat pumps with extended operating window • new working media and compressors, gaseous working media
Power to hydrogen	cost reduction factor 2 for alkaline electrolysers	• Improvement of stack and system engineering, and manufacturing • increased current density at cell level • catalysts with improved current exchange; rates, controlled morphologies and physicochemical properties and high stability in alkaline environments. • membranes with lower gas cross-over rates and increase lifetime • demonstration of multi-MW scale alkaline electrolysers with reduced footprint and greater ease of commissioning and operation
	Cost reduction factor 4 for polymer electrolyte membrane (PEM) electrolyser systems	• Cost reduction or substitution of bipolar flow field plates representing ~50% of stack costs; advanced coatings or plate manufacturing techniques • design of flow field-free bipolar plates use of large cell areas (0.5m² and more) • Maximise active cell area to reduce specific material cost thermal management, and uniform current distribution at high current densities.

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[130] BIC Strategic Innovation and Research Agenda (SIRA) -Bio-based and Renewable Industries for Development and Growth in Europe; http://biconsortium.eu/sites/biconsortium.eu/files/downloads/BIC_BBI_SIRA_web.pdf

		• Advanced catalysts for the OER (oxygen evolution reaction) electrode with high corrosion resistance and catalytic activity; reduced noble metal loadings (issue with Iridium due to high cost and potential future supply); advanced catalyst support structures, mixed metal oxides and nanostructured catalysts • Alternative/ advanced membrane materials and fabrication techniques (currently 5% of stack cost); improve ion exchange characteristics and mechanical stability. • Advanced catalysts for the HER (hydrogen evolution reaction) electrode; reduce loadings or replace noble metals
	Performance and cost reduction in Alkaline membrane (AEM) electrolysis	• Improve ion conductivity of the membrane,, as this currently limits AEM to current densities below 0.5 A/cm².
	Performance and cost reduction in solid oxide electrolysis (SOE)	• Development of corrosion- and high temperature resistant materials and seals • Improve cell and stack design, proof of Life time, cycling stability • Demonstrate full system operation • Review and analyse the business case for co-electrolysis and other novel use cases enabled by SOE high temperature operation
	Operational flexibilityof electrolysis	• Optimisation of system components for quick response to load changes • Stack design, optimisation of pumps, gas-water separators, and pressure control for fast-ramping regimes. • Increased cell efficiency when operating in part load mode (through lower current density), minimisation of parasitic loads in the system components • Investigation of impacts on lifetime caused by dynamic operation
Alternative hydrogen production	Methane pyrolysis as alternative	• Investigation of pathways, i.e. thermal decomposition, plasma pyrolysis thermocatalytic decomposition or liquid metal processes
	Water photolysis as long term option	• water photolysis in lab scale: development of highly efficient (performance), corrosion-resistant (longevity) photoelectrode materials and processing technologies; development of electrodes without noble metals and other rare elements and with reduction >50% of overpotential in H2
	Thermochemical processes and CSP	• Investigate the use for high-temperature industrial waste heat • New reactor concepts, efficient and robust reactor designs compatible with high temperatures and heat cycling • New catalytic thermochemical cycles to reduce temperature

		requirement • Increase efficiency and durability of reactant materials for thermochemical cycling • .For solar thermochemical systems, reduce cost of the concentrating mirror systems
Power to chemicals	Co-electrolysis	• Investigation of co-electrolysis of CO_2 and water in SOE to syngas
	Electrochemical processes	• Investigation of electrochemical processes based on new materials and a better understanding of electrochemistry • Use of operating parameters, such as temperature, pressure and pH, to influence the reactions and improve activity and selectivity. • Enable product flexibility that can help improving the business case for power-to- chemicals
	Methanol production from CO_2 and hydrogen	• Improvement of productivity; development of novel catalysts less sensitive to inhibition by high concentration of CO_2 and H_2O to improve productivity; • Explore small scale systems e.g. coupled to biogas plants with fast start/shut-down operations • Increase scale of demo plants and build up operation experience
	Ammonia production from hydrogen	• Investigate hybrid concepts with flexible operation based on both electricity and NG • Optimized concepts for heat generation and heat integration, process integration with subsequent urea synthesis also for hydrogen based ammonia plants
	Direct electrocatalytic ammonia production (long term)	• direct electrocatalytic or photocatalytic ammonia production process in which nitrogen reduction reaction catalysts are employed to directly produce ammonia, with OER catalysts balancing the reaction by oxidizing water to produce the protons and electrons needed for the nitrogen reduction
	Electrochemical reduction of CO_2 (emerging)	• Electrochemical reduction of CO_2 to formic acid; ;process concepts incl. cost-effective solutions to concentrate formic acid solutions • Direct electrocatalytic conversion of CO_2 to ethylene • General: catalysts with long-term performance characteristics and low energy use; reactor configurations, scale up.high productive catalysts not based on noble metals; improve catalyst stability and productivity
	Alternative energy supply	• Investigate technologies other than electrochemical pathways, such as plasma, microwave and photocatalysis, which might lead to higher energy efficiencies and product yields by

		activating the molecules in different ways than electrochemistry or conventional thermochemical processes
Biomass to chemicals and materials	Pretreatment of lignocellulosic biomass	• Demonstration of cost-effective fractionation, separation and purification technologies for lignocellulosic biomass into its basic components, such as lignin, cellulose, hemi-cellulose, sugars and other carbohydrates
	Cost and resource efficient production	• Improving the overall conversion yield from the lignocellulosic feedstock into biochemicals and biofuels • innovative biotechnological, biocatalytic and catalytic routes to obtain building blocks and chemicals from cellulosic sugars (C5 and C6) • Demonstrate the economics of combined production of biofuels and bio-based chemicals from lignocellulosic feedstock at large scale
	Bioethanol from lignocelluloses	• Gasification and subsequent fermentation or chemo-catalytic conversion of synthesis gas by means of MoS_2-based catalysts
	Aromatics from lignocellulosis and lignin	• Selective pyrolysis/ catalytic fast pyrolysis of lignocelulosis to aromatics or hydrogenation of lignin to depolymerize the complex lignin structure and stabilize reactive intermediates
	Bio-based materials	• Develop and demonstrate new functional bio-based materials: e.g. bioplastics, biocomposites, materials based on lignin, starch, (nano-)cellulose or carbon fibre: towards fit-for-purpose solutions for diverse industrial customers
	Integrated biorefineries	• Integrating the production of bio-products and advanced bio-energy carriers in a smart way (smart use, maximise carbon and energy yield from biomass)
Alternative chemical production	Ammonia	• Solid state ammonia synthesis using proton-conducting membranes • Solar thermochemical loopingfor ammonia production (long term); new alloys and doped materials and to achieve process integration and optimization for the N_2 activation through metal nitridation/reduction cycles using heat/photons generated by solar thermal processes. • Biochemical routes, enzyme catalysts for N_2 reduction to ammonia (long term); functional immobilization of recalcitrant redox enzymes, including nitrogenase, on electrode surfaces
	Olefins	• Direct electrocatalytic conversion of CO_2 to ethylene • direct Fischer-Tropsch to Olefin (FTO); conversion of CO_2/H_2 to light olefins using modified Fischer–Tropsch catalysts
Circular economy and	Secondary raw materials	• Utilisation and valorisation of secondary feedstocks like residue and waste streams and recycled end-of-life materials

industrial sym-biosis		• Polymer waste: pre-processing catalytic cracking and plasma gasification • Development and demonstration of new functional bio-based chemicals and materials from side streams and residues from forestry and pulp and paper mills (e.g. based on lignin, cellulose, or e.g.hemicelluloses) • LCA of secondary feedstock to product chains

13 Policy measures

Despite the reasonably high maturity of the technologies described in this study, two main barriers can be identified, which hamper the fast implementation of these technologies:

- The economic gap compared to conventional, fossil production; this is valid for both renewable hydrogen and biomass-based production pathways; power costs (in the case of electricity based processes) and renewable feedstocks (for bio-based processes) are not competitive at current low costs of fossil feedstocks. Even if this situation changes in the near future, the high volatility of prices will seriously hamper large investment decisions.
- Manufacturing experience and prove of concept on a large industrial scale is missing; this is particularly true for the hydrogen and CO_2-based routes, but also for emerging biomass routes and an expected shift towards lignocellulosic biomass. Necessary technologies for all proposed production pathways are available in principle, and demonstration plants are in operation, but more reference cases are needed, in which these technologies have been combined on an industrial scale. Hence, operational experience and reliable cost evaluations on production scale are missing.

Policy measures will have an important role in removing these barriers and facilitating the deployment of low-carbon technologies using several mechanism:

- Ensuring availability and competitive access to low-carbon electricity;
- Funding of research and innovation including pilot and demonstration activities to further advance key technologies and to prove and demonstrate cross-sectorial collaboration models;
    - Provide long-term funding commitments from various public and private sources are necessary to ensure a continuity of research and innovation programmes,
    - Open funding instruments and strategic initiatives to new low-carbon technologies,
    - Support the development of Public-Private-Partnerships (PPPs) to focus RD&I efforts and to enable risk sharing for investments for demonstration of innovative technologies; a cross-sectorial view is beneficial, hence partnerships should cover relevant sectors to facilitate industrial symbiosis. The PPP SPIRE is a role model for this.
- Support and information accompanying the development of technology options;
    - Ensure dedicated LCA studies based on an appropriate methodology on emerging low-carbon technologies including circular economy and industrial symbiosis set-ups,

providing proven data for well defined cases. This data should also provide evidence in terms of the sustainability of biofuels and synthetic fuels that form the basis of an enhanced low-carbon fuel quota. All data should be made available in a central register for all

- Support the establishment of a central database of sources and infrastructures for Europe, including biomass, CO_2 and other gaseous effluent sources to support industrial symbiosis. Emitters should be included that are lower than the minimum 10000 tons per annum threshold for reporting to the European Pollutant Release and Transfer Register.
- The options should be considered in IEA roadmaps and EU scenarios on a low carbon economy, stimulating appropriate policy frameworks considering these options.

14 Transformation of the European Chemical Industry

The chemical industry has long been subject to profound changes in its energy supply and feedstock base. Within the chemical industry, and in marked contrast to other energy-intensive industries, fossil-based fuels act in both functions, providing carbon and energy as raw materials, i.e. feedstocks, as well as serving more conventional energy supply functions, like supplying heat. The scenarios within this study aim towards a more sustainable European chemical industry, which require significant changes of the current fossil-based chemical industry towards a renewable feedstock base and energy supply.

14.1 Current energy supply, feedstock base and carbon-flows of the European chemical industry

The processes discussed in this study are the backbone of the European chemical industry. For the processes investigated in this study, the current energy flows are depicted in Figure 45. It is predominantly based on naphtha as principal feedstock to produce the so-called “high-value chemicals” (HVCs), which in turn are raw materials for numerous chemical transformations. The second largest contribution comes from natural gas which is mainly utilized in the production of ammonia. Direct utilization of electricity and heavy oil are far more limited. The former is predominantly used in the production of chlorine while the latter is used in methanol synthesis.

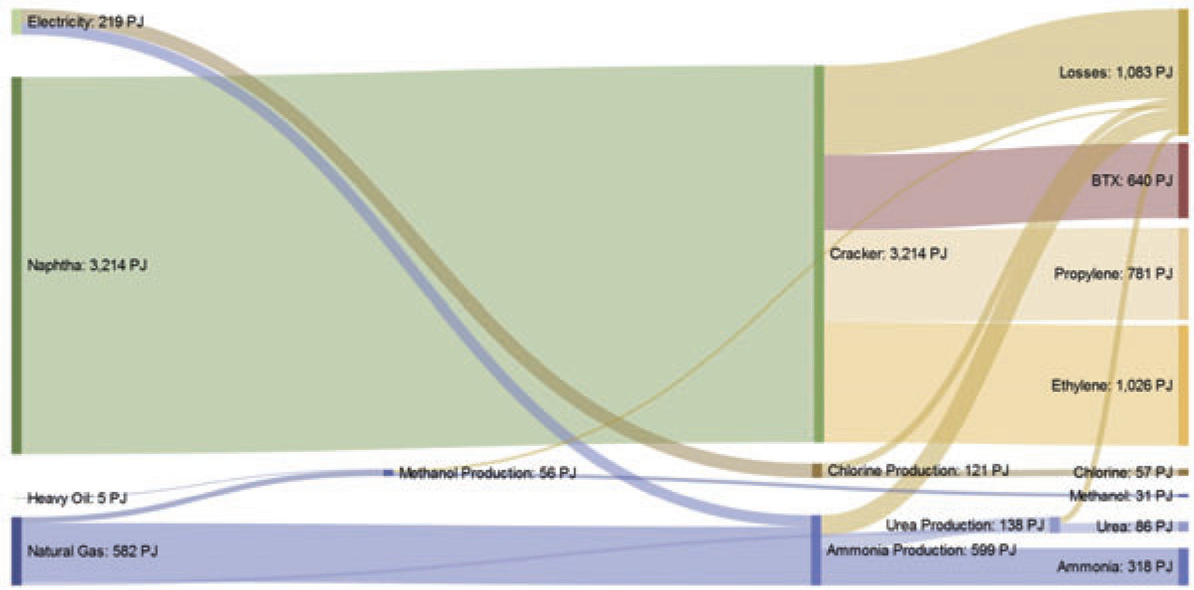

Figure 45: Energy-flow diagram of the current state (2015) of the processes under consideration

The corresponding carbon flows are depicted in Figure 46 as "CO_2 flows", i.e. the amount of CO_2 emitted in stoichiometric combustion of the compound. The actual emissions caused by the processes under investigation are shown as emissions on the right-hand side of the diagram. Chlorine and ammonia do not have carbon content and are depicted with an arbitrarily 0.1 million tons of CO_2 attributed in order to make them visible within the diagram.

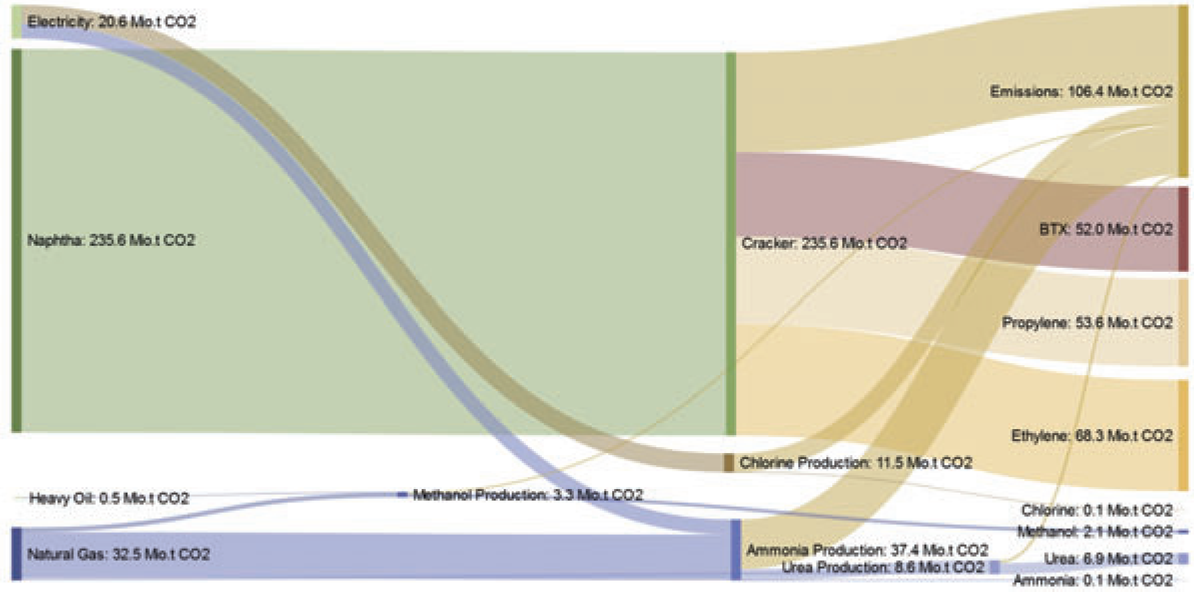

Figure 46: Carbon-flow diagram for the current state (2015) of the processes under consideration

14.2 Energy supply, feedstock base and carbon-flows of the European chemical industry in the BAU scenario

Within the “business-as-usual” scenario for 2050 (BAU 2050), the processes under consideration are unaltered, and so are the feedstock and energy supplies. Two dominant effects are visible: an increased production volume of 1 % p.a. leads to a corresponding increase in fuel and feed demand, while the decarbonisation efforts within the power sector significantly reduce the amount of emissions attributed to the use of electricity to an extent, that chlorine production becomes effectively emission-free. The energy-flow and carbon-flow diagrams are respectively shown in Figure 47 and Figure 48.

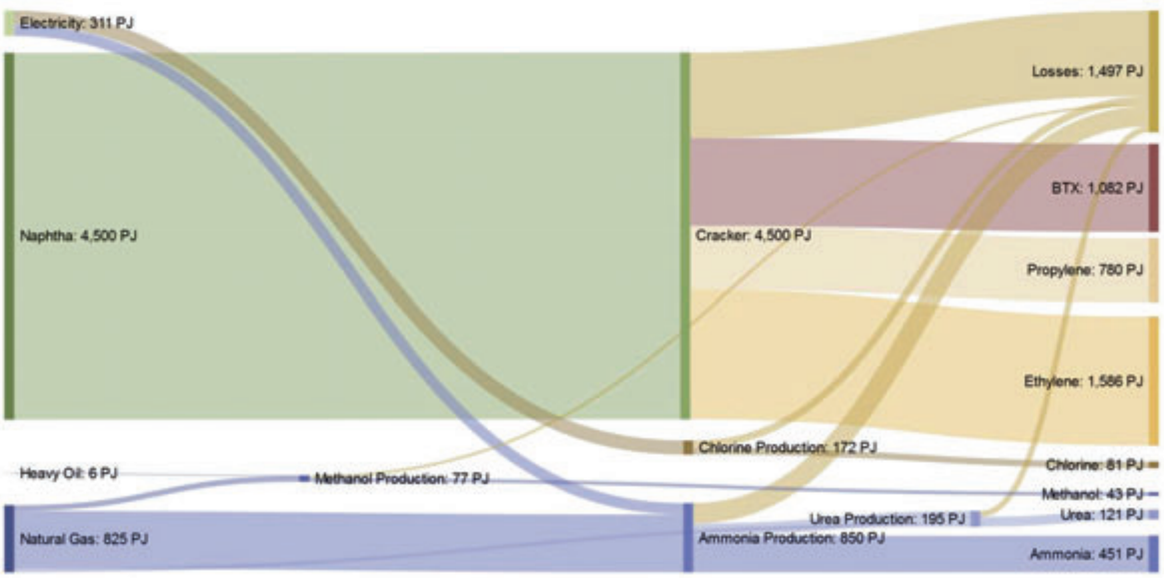

Figure 47: Energy-flow diagram of the processes under consideration in 2050 within the BAU scenario

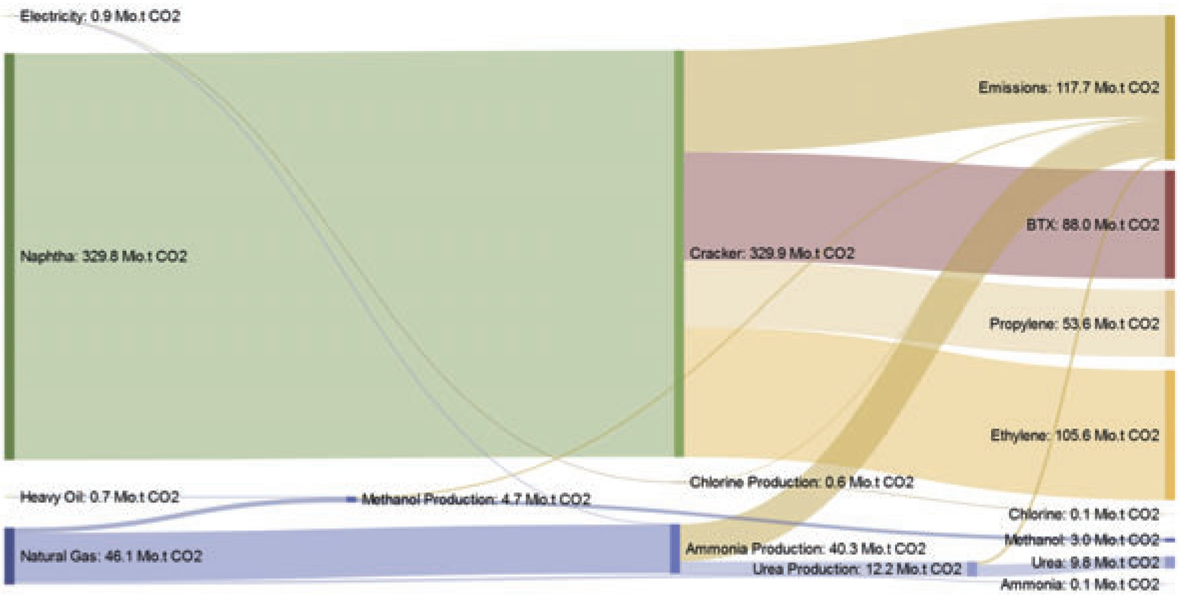

Figure 48: Carbon-flow diagram of the processes under consideration in 2050 within the BAU scenario

Applying efficiency measures, Figure 49 and Figure 50, does not change the relative contributions of energy and feed significantly but reduces the overall energy and carbon requirement by around 5 % compared to BAU 2050 without efficiency measures. Compared to the current state of the processes under consideration, the BAU 2050 scenario predicts an increase of nearly 40% in energy and feed consumption, as well as an increase in CO_2 emissions of 11%. Applying efficiency measures reduces the increase in energy and feed requirements by 33% while leading to an overall reduction in emissions of nearly 5%.

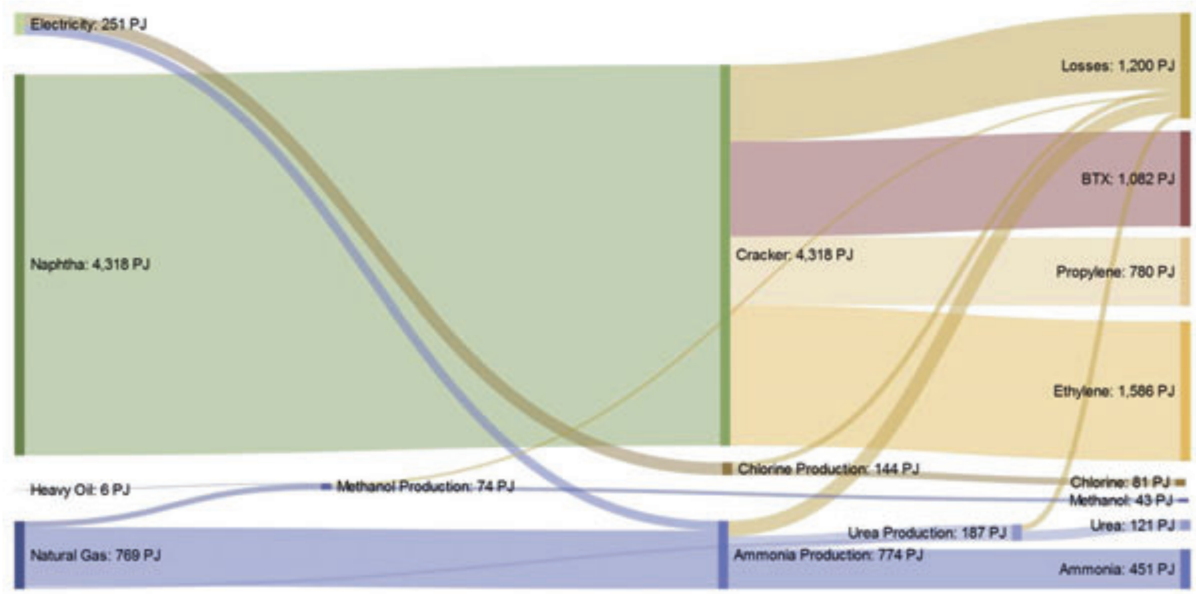

Figure 49: Energy-flow diagram of the processes under consideration in 2050 within the BAU scenario with efficiency measures

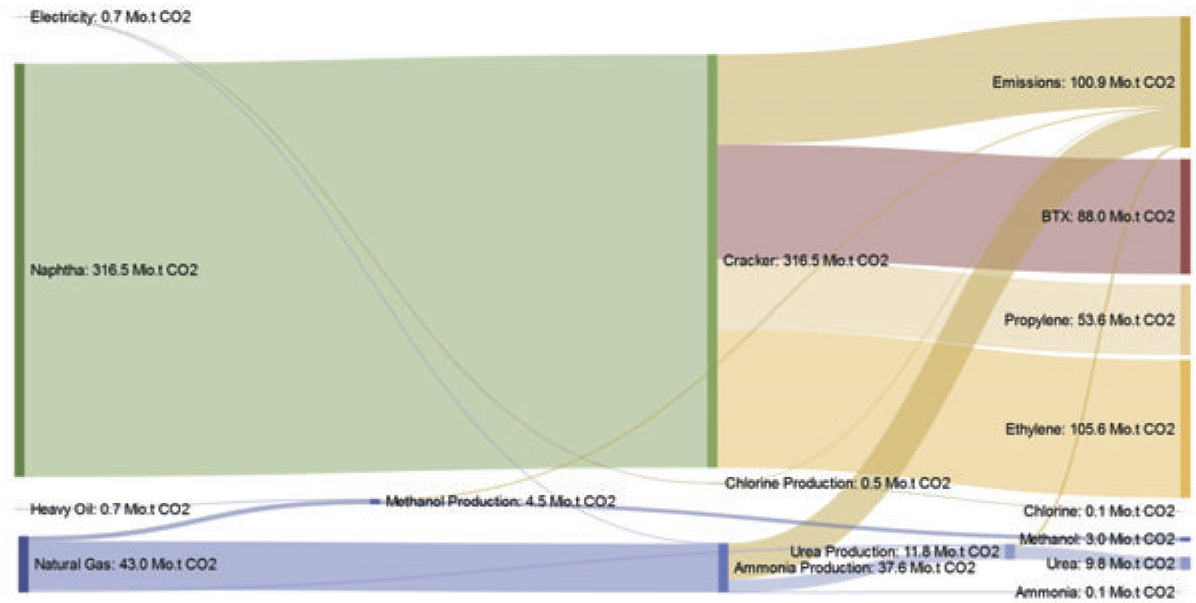

Figure 50: Carbon-flow diagram of the processes under consideration in 2050 within the BAU scenario with efficiency measures

14.3 Energy supply, feedstock base and carbon-flows of the European chemical industry in the Intermediate scenario

In 2050 the intermediate scenario reaches a deployment of 35% of low-carbon technologies while all plants and processes are subject to efficiency improvements and the European production volume expands by 1% p.a. As a result, there is a significant shift in the energy and feedstock base towards electricity, which contributes 30% to the energy and feedstock input, as well as an increase of the overall energy requirement due to hydrogen (labeled "electricity feed") production via electrolysis of nearly 60% compared to the status quo, see Figure 51. Electricity consumption for these processes reaches the order of current gross electricity production in Germany. Methanol becomes a central platform chemical that starts replacing the classical steam cracking process and contributes to the production of HVCs and BTX, while naphtha consumption is reduced. These shifts can still be implemented by deploying low-carbon technologies via retrofitting existing plant capacity and capacity extensions.

There is also a significant shift within the feedstock base with CO_2 becoming a carbon source within the European chemical industry, as shown in Figure 52. These processes overall are still net emitters of CO_2 within this scenario but can accommodate around 65% of its emissions as new feedstock.

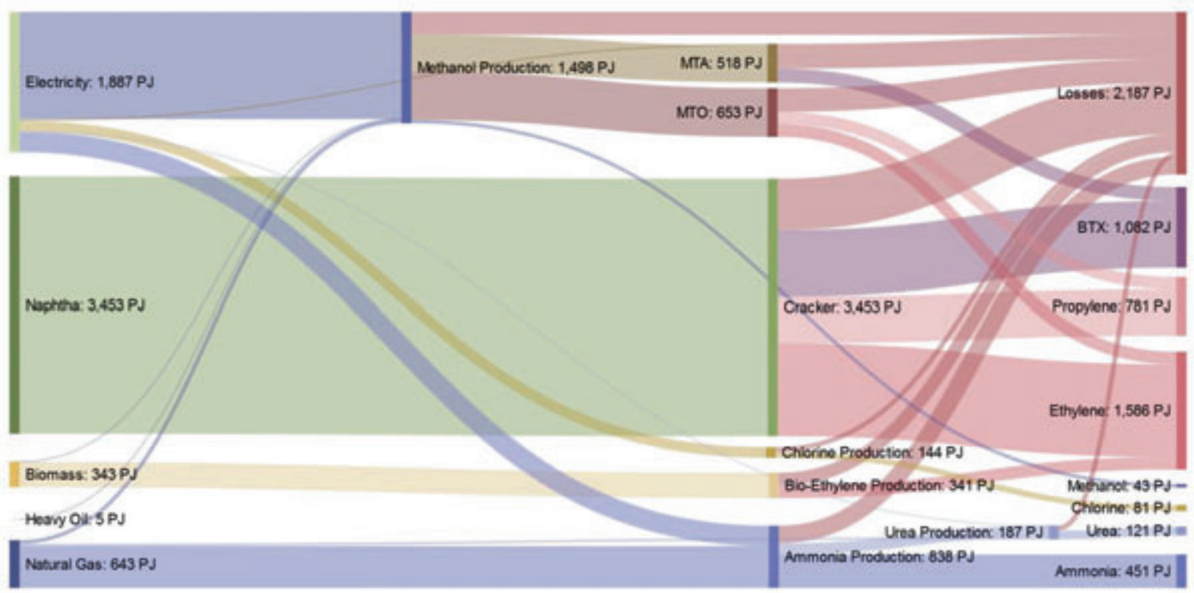

Figure 51: Energy-flow diagram of the processes under consideration in 2050 within the Intermediate scenario

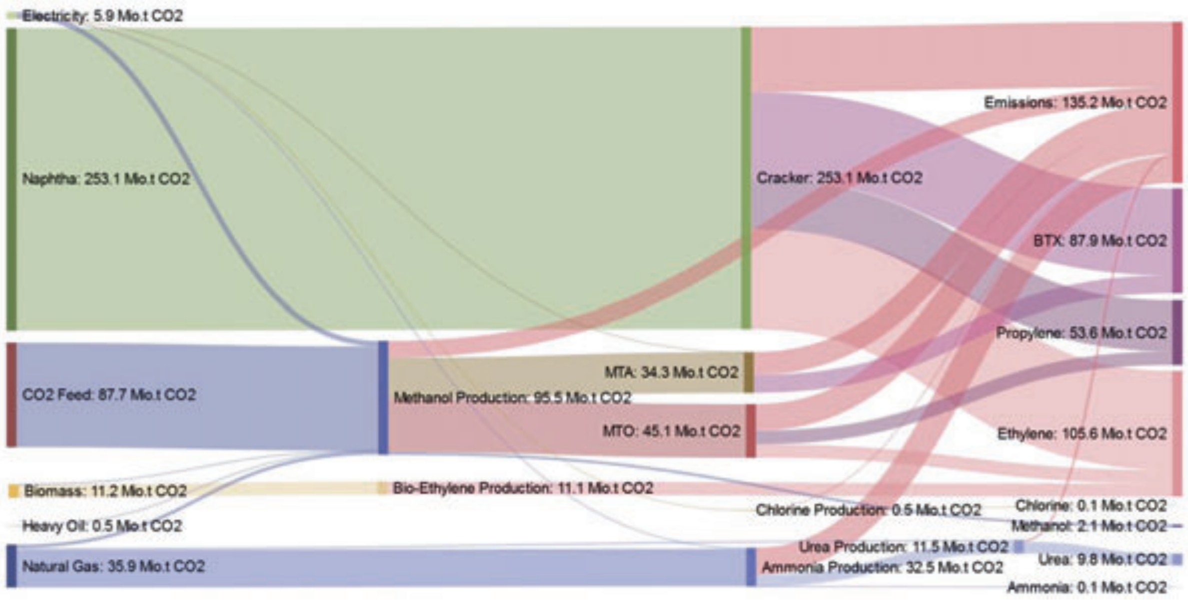

Figure 52: Carbon-flow diagram of the processes under consideration in 2050 within the Intermediate scenario

14.4 Energy supply, feedstock base and carbon-flows of the European chemical industry in the Ambitious scenario

Similar to the developments in the Intermediate scenario, the Ambitious scenario aims at an even higher rate of implementation of low-carbon processes to reach 50% by 2050, see Figure 53. This value can no longer be reached by simply deploying new technology when capacity extension takes place, rather it requires conventional plants being actively decommissioned at replaced by new technology-based plants at a rate of 0,75% p.a. in addition to deploying it to all new and retrofitted capacity. Electricity becomes the main energy vector for producing methanol in order to generate HVCs to enter the chemical industry's value chains. Electricity consumption of the processes under consideration is in the order of 1.5 times of the current gross electricity production in Germany. Overall energy consumption increases by 80% compared to 2015. Naphtha consumption is reduced to about 80% of the current level.

The use of CO_2 as carbon source overtakes naphtha as feedstock (Figure 54) and the European chemical industry becomes a net consumer of CO_2 albeit still emitting about 60% more CO_2 than in 2015.

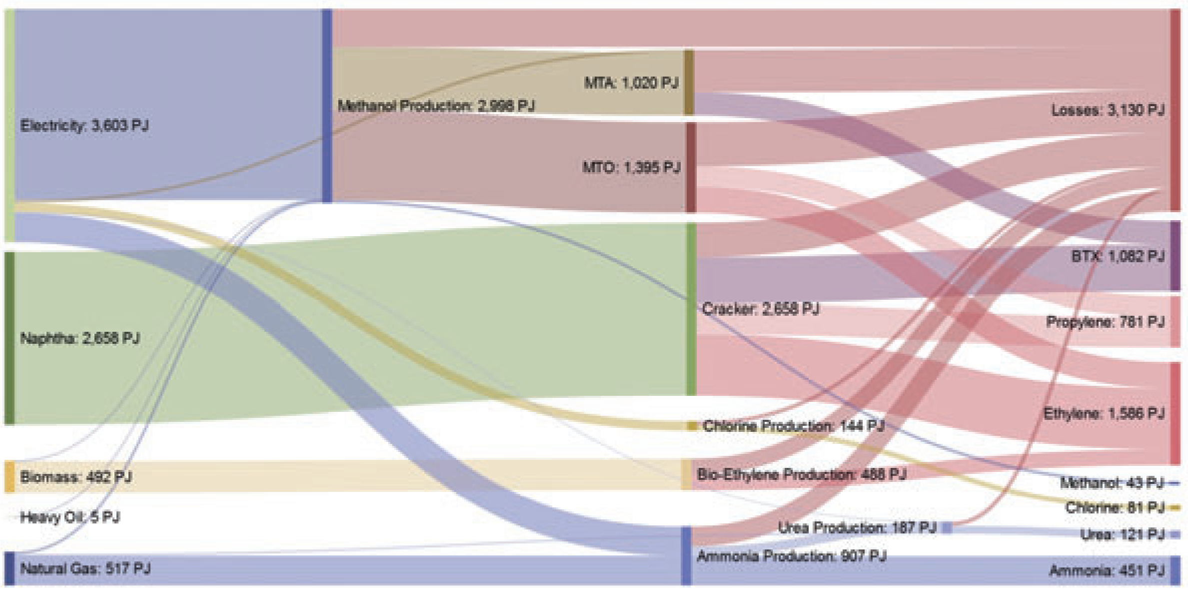

Figure 53: Energy-flow diagram of the processes under consideration in 2050 within the Ambitious scenario

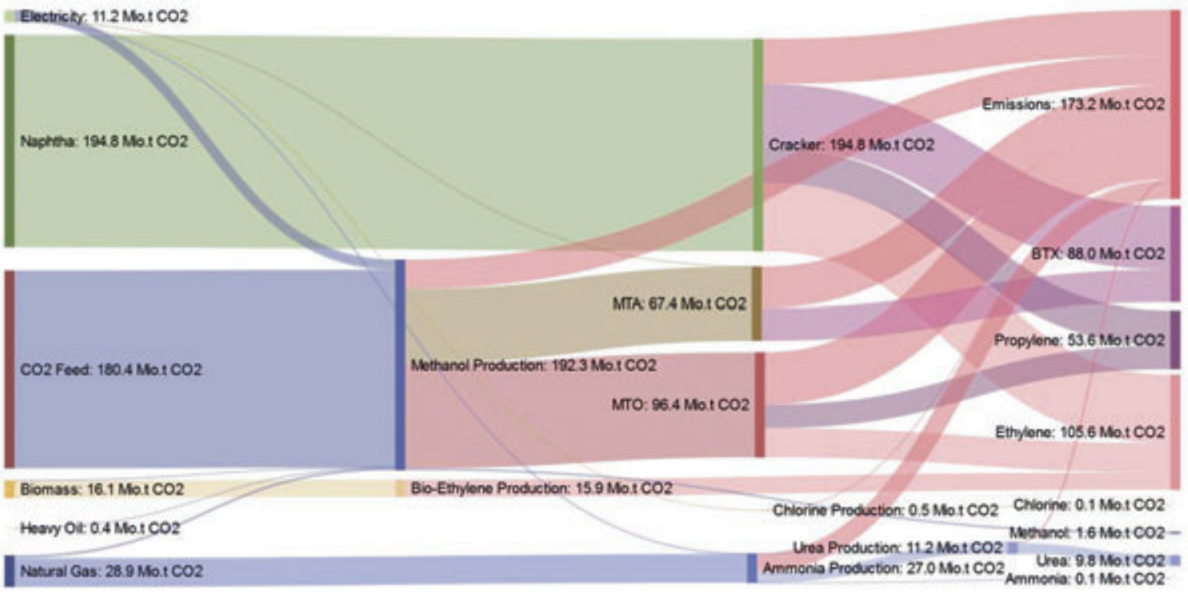

Figure 54: Carbon-flow diagram of the processes under consideration in 2050 within the Ambitious scenario

14.5 Energy supply, feedstock base and carbon-flows of the European chemical industry in the Maximum scenario

The maximum scenario depicts the complete transformation of the processes covered by this study towards low-carbon technologies. This transformation requires active decommissioning of existing conventional plants and replacement by new technologies at a rate of around 3% in addition to all capacity extension and retrofitting being new technologies. Energy supply is dominated by electricity and natural gas only, see Figure 55, and extends to 2.5 times the current energy consumption. The latter is used for distillation of methanol, which acts as platform to produce HVCs and has completely replaced conventional steam cracking. Electricity consumption of these processes approaches the current electricity generation in the European Union.

For these processes, CO_2 becomes the dominant source of carbon, as shown in Figure 56 for all transformations, making these processes net consumers in the order of around 200 million tons of CO_2.

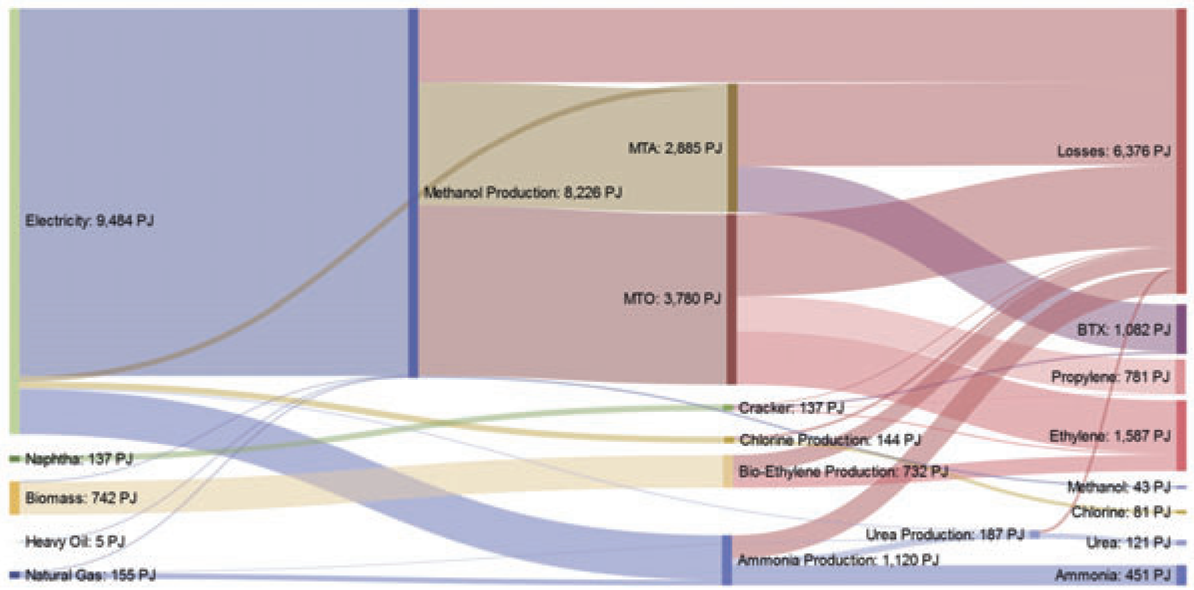

Figure 55: Energy-flow diagram of the processes under consideration in 2050 within the Maximum scenario

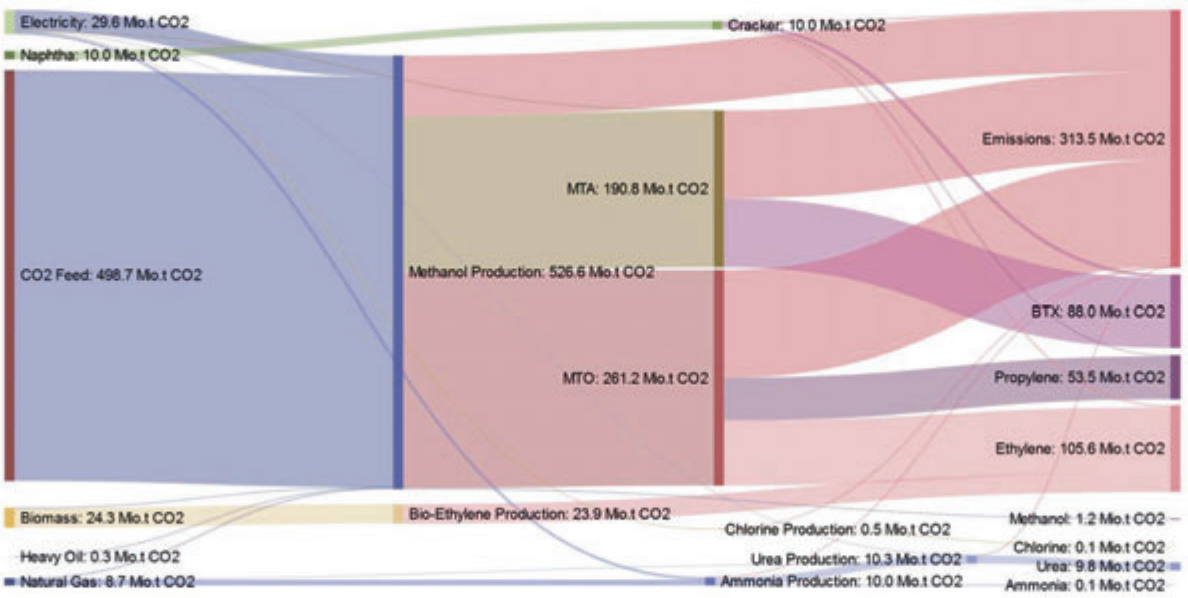

Figure 56: Carbon-flow diagram of the processes under consideration in 2050 within the Maximum scenario

15 Acknowledgement

The study project team would like to thank all experts that contributed generously to this study with their knowledge, experience and viewpoints. In particular, we would like to express our gratitude to all participants in two validation workshops on 23 September 2016 and 8 November 2016 in Brussels, representing the following companies: AkzoNobel, BASF, Clariant, Dow Benelux, Evonik, Exxon Mobil Chemical, Solvay, Repsol and Total. The discussions of results and assumptions in these meetings, in which the authors presented initial facts and findings, have been very constructive and helpful. Many of these experts additionally served as reviewers of the draft report, and the project team appreciates the effort dedicated and the numerous improvement suggestions.

The author's team at DECHEMA:	The project supervisors at Cefic:
Alexis Bazzanella	Pierre Barthelemy
Florian Ausfelder	Sophie Wilmet

16 Annexes

Annex 1: Assumptions for calculation of hydrogen cost as function of the operating hours

Technology	Power/Capacity min /MW	Power max /MW	Efficiency, min	Efficiency, max	Investment, low	Investment, high
Alkaline Electrolyzer	20	150	65%	82%	850	1500
PEM Electrolyzer	0.15	1	65%	78%	1300	3800

Electricity costs for the calculation of production costs are set to 40 €/MWh throughout the study.

Annex 2: Assumptions scenario work

Assumptions	Scenario	2020	2025	2030	2035	2040	2045	2050
Share H_2-based MeOH, olefin, BTX plants	Max	5%	10%	20%	40%	60%	75%	85% (BTX 100%)
	Amb	1%	5%	10%	15%	20%	30%	50%
	Interm	1%	2,5%	5%	7.5%	15%	23%	30%
Share biomass based MeOH, olefins	Max	1%	2%	3%	4%	5%	10%	15%
	Amb	1%	2%	3%	4%	5%	7.5%	10%
	Interm	1%	2%	3%	4%	5%	6%	7%
Share MeOH in gasoline	Max	5%	10%	20%	30%	45%	70%	96.5%
	Amb	1%	5%	10%	15%	20%	30%	40%
	Interm	1%	2.5%	5%	7.5%	10%	15%	20%
Share synthet. Jetfuels, syndiesel	Max	5%	10%	20%	30%	45%	70%	100%
	Amb	1%	5%	10%	15%	20%	30%	40%
	Interm	0.5%	1.0%	2.5%	5%	7.5%	10%	15%
Share bioethanol	All	0.6%	0.8%	1%	1.3%	1.8%	2.7%	3.5%
Plant replacement rate	Max	14%	29%	43%	57%	71%	86%	100%
	Amb	8%	15%	23%	30%	38%	45%	53%
	Interm	5%	10%	15%	20%	25%	30%	35%
Electric steam generation and steam recompression	All	0%	2%	5%	15%	30%	50%	70%
Efficiency measures	All	0.56% p.a.						

Annex 3: Annual assumptions, impact and demand figures for the intermediate scenario

	Pathways total	2015	2020	2025	2030	2035	2040	2045	2050
Production	MeOH via H_2, fuel [mill. t]	0	2	3	6	8	8	9	10
	Bioethanol, fuel [mill. t]	0,00	0,35	0,37	0,39	0,41	0,43	0,45	0,48
	Syn. Jetfuel [mill. t]	0,00	0,25	0,45	0,99	1,68	2,37	3,03	4,49
	Syndiesel [mill. t]	0	1	1	3	5	7	8	10
	MeOH via H_2 chem. [mill. t]	0,00	0,16	0,62	2,13	4,58	12,04	22,57	36,36
	Olefins via H_2 to MeOH [mill. t]	0,00	0,03	0,13	0,44	0,94	2,43	4,52	7,21
	BTX, via MeOH [mill. t]	0,00	0,02	0,07	0,25	0,56	1,48	2,79	4,54
	Ammonia via H_2 [mill. t]	0	0,0	0,1	0,2	0,5	1,2	2,3	3,7
	Urea via H_2 to NH_3; [mill. t]	0	0,0	0,0	0,1	0,3	0,7	1,3	2,0
	Chlorine [mill. t]	9,58	10,07	10,58	11,12	11,69	12,28	12,91	13,57
	MeOH, bio-based [mill. t]	0,00	0,00	0,00	0,01	0,02	0,04	0,05	0,05
	Olefins, bio-based [mill. t]	0,00	0,40	0,83	1,30	1,80	2,34	2,92	3,55
	BTX, bio-based [mill. t]	0	0	0	0	0	0	0	0
Avoided CO_2	MeOH, fuel [mill. t]	0,0	2,3	5,0	8,8	11,3	11,9	13,0	14,5
	Bioethanol, fuel [mill. t]	0,0	0,7	0,7	0,7	0,8	0,8	0,8	0,9
	Syn. Jetfuel [mill. t]	0,0	0,5	0,8	1,8	3,1	4,4	5,6	8,3
	Syndiesel [mill. t]	0,0	1,9	3,4	7,2	12,5	16,6	18,8	23,9
	MeOH via H_2, chem. [mill. t]	0,0	0,0	0,0	0,0	0,1	0,2	0,3	0,5
	Olefins via H_2 to MeOH [mill. t]	0,0	0,1	0,3	0,8	1,8	4,6	8,6	13,7
	BTX, via H_2 to MeOH [mill. t]	0,00	0,03	0,12	0,43	0,95	2,52	4,76	7,73
	NH_3 via H_2 [mill. t]	0,0	0,0	0,1	0,4	0,8	2,1	3,9	6,3
	Urea via H_2 to NH_3 [mill. t]	0,0	0,0	0,0	0,1	0,2	0,5	0,9	1,5
	MeOH, bio-based [mill. t]	0,00	0,00	0,01	0,01	0,03	0,04	0,05	0,06
	Olefins, bio-based; [mill. t]	0,00	0,99	2,05	3,19	4,42	5,75	7,18	8,73
	BTX, bio-based [mill. t]	not included							
Electricity demand	MeOH fuel [TWh]	0	17	38	67	86	91	98	110
	Syn. Jetfuel [TWh]	0	16	28	62	105	148	190	282
	Syndiesel [TWh]	0	53	94	198	341	454	515	655
	MeOH chem. [TWh]	0,0	0,0	0,1	0,2	0,5	1,2	2,3	3,6
	BTX [TWh]	0,0	1,0	3,4	12,1	26,4	70,2	132,8	215,6
	Olefins [TWh]	0	2	10	33	70	180	335	535
	NH_3 [TWh]	0,0	0,2	0,8	2,8	5,9	15,5	28,8	46,0
	Chlorine [TWh]	45	42	41	40	40	39	38	38
	Steam generation [TWh]	0,0	2,0	5,2	16,2	33,3	57,2	82,5	121,4
	Steam recompr. [TWh]	0,0	0,0	0,1	0,2	0,3	0,6	0,8	1,2
	Carbon free electricity 2DS [TWh]	1670	2002	2337	2656	2920	3087	3254	3367
	% of carbon-free electricity (IEA2DS)	3%	7%	9%	16%	24%	34%	44%	60%
Required CO_2	MeOH as fuel, CO_2 [mill. t]	0	2	5	8	11	11	12	14
	Syn. Jetfuel, CO_2 [mill. t]	0	1	1	3	5	7	10	14
	Syndiesel, CO_2 [mill. t]	0	3	5	10	17	23	26	33
	MeOH chem., CO_2 [mill. t]	0,0	0,0	0,0	0,0	0,1	0,2	0,3	0,5
	BTX, CO_2 [mill. t]	0,0	0,1	0,4	1,5	3,3	8,7	16,5	26,9
	Olefins, CO_2 [mill. t]	0,00	0,10	0,42	1,39	2,94	7,64	14,17	22,62
	Urea, CO_2 [mill. t]	0	0,0	0,03	0,09	0,19	0,50	0,92	1,48
	Olefins, required MeOH [mill t]	0,00	0,08	0,31	1,01	2,14	5,56	10,32	16,47
Required biomass	MeOH, bio-based [mill. t]	0,00	0,06	0,19	0,48	0,91	1,48	1,83	2,20
	Bioethanol, fuel [mill. t]	89	94	96	98	95	84	72	59
	Olefins, bio-based; [mill. t]	0,00	4,22	8,75	13,63	18,88	24,54	30,64	37,24
	BTX, bio-based [mill. t]	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00

	Avoided CO2 incl. efficiency	2015	2020	2025	2030	2035	2040	2045	2050
Efficiency and steam	Chemicals [mill t]	0,0	0,1	0,5	1,8	3,8	9,9	18,5	38,5
	Fuels [mill t]	0,0	5,4	10,0	18,6	27,6	33,7	38,2	47,6
	Efficiency measures [mill t]	0,00	1,91	3,76	5,42	6,98	8,16	9,21	10,04
	Electricity based steam [mill t]	0,00	0,34	0,89	2,74	5,65	9,69	13,95	20,49
	Steam recompression [mill t]	0,00	0,03	0,08	0,27	0,59	1,02	1,48	2,19

Annex 4: Annual assumptions, impact and demand figures for the Amb scenario

Pathways total		2015	2020	2025	2030	2035	2040	2045	2050
Production	MeOH via H_2, fuel [mill. t]	0	2	7	12	16	16	18	20
	Bioethanol, fuel [mill. t]	0,00	0,35	0,37	0,39	0,41	0,43	0,45	0,48
	Syn. Jetfuel [mill. t]	0,00	0,51	2,26	3,95	5,04	6,31	9,09	11,97
	Syndiesel [mill. t]	0	2	7	13	16	19	25	28
	MeOH via H_2 chem. [mill. t]	0,00	0,20	1,64	5,45	11,53	20,00	37,19	74,41
	Olefins via H_2 to MeOH [mill. t]	0,00	0,04	0,37	1,18	2,46	4,22	7,77	15,41
	BTX, via MeOH [mill. t]	0,00	0,02	0,18	0,63	1,35	2,36	4,43	8,93
	Ammonia via H_2 [mill. t]	0	0,0	0,2	0,6	1,2	2,1	3,8	7,6
	Urea via H_2 to NH_3; [mill. t]	0	0,0	0,1	0,3	0,7	1,1	2,1	4,2
	Chlorine [mill. t]	9,58	10,07	10,58	11,12	11,69	12,28	12,91	13,57
	MeOH, bio-based [mill. t]	0,00	0,00	0,01	0,02	0,03	0,05	0,09	0,14
	Olefins, bio-based [mill. t]	0,00	0,40	0,83	1,30	1,80	2,34	3,65	5,06
	BTX, bio-based [mill. t]	0	0	0	0	0	0	0	0
Avoided CO_2	MeOH, fuel [mill. t]	0,0	2,3	10,1	17,6	22,6	23,9	26,0	29,1
	Bioethanol, fuel [mill. t]	0,0	0,7	0,7	0,7	0,8	0,8	0,8	0,9
	Syn. Jetfuel [mill. t]	0,0	0,9	4,2	7,3	9,3	11,7	16,8	22,1
	Syndiesel [mill. t]	0,0	3,9	17,1	28,9	37,4	44,2	56,4	63,8
	MeOH via H_2, chem. [mill. t]	0,0	0,0	0,0	0,1	0,2	0,3	0,5	1,1
	Olefins via H_2 to MeOH [mill. t]	0,0	0,1	0,7	2,2	4,7	8,0	14,7	29,2
	BTX, via H_2 to MeOH [mill. t]	0,00	0,04	0,31	1,07	2,30	4,03	7,55	15,23
	NH_3 via H_2 [mill. t]	0,0	0,0	0,3	1,0	2,1	3,5	6,5	13,0
	Urea via H_2 to NH_3 [mill. t]	0,0	0,0	0,1	0,2	0,5	0,8	1,6	3,1
	MeOH, bio-based [mill. t]	0,00	0,00	0,01	0,02	0,03	0,05	0,10	0,16
	Olefins, bio-based; [mill. t]	0,00	0,99	2,05	3,19	4,42	5,75	7,80	9,56
	BTX, bio-based [mill. t]	not included							
Electricity demand	MeOH fuel [TWh]	0	17	76	133	171	181	197	220
	Syn. Jetfuel [TWh]	0	32	142	248	316	396	570	751
	Syndiesel [TWh]	0	106	469	790	1024	1211	1545	1748
	MeOH chem. [TWh]	0,0	0,0	0,2	0,6	1,2	2,0	3,8	7,5
	BTX [TWh]	0,0	1,1	8,7	29,8	64,0	112,3	210,6	424,6
	Olefins [TWh]	0	3	29	92	192	330	608	1206
	NH_3 [TWh]	0,0	0,3	2,2	7,2	15,1	26,0	48,1	95,5
	Chlorine [TWh]	45	42	41	40	40	39	38	38
	Steam generation [TWh]	0,0	2,0	5,2	16,2	33,7	58,8	86,8	131,2
	Steam recompr. [TWh]	0,0	0,0	0,1	0,2	0,3	0,6	0,9	1,3
	Carbon free electricity 2DS [TWh]	1670	2002	2337	2656	2920	3087	3254	3367
	% of carbon-free electricity (IEA2DS)	3%	10%	33%	51%	64%	76%	102%	137%
Required CO_2	MeOH as fuel, CO_2 [mill. t]	0	2	9	17	21	23	25	27
	Syn. Jetfuel, CO_2 [mill. t]	0	2	7	12	16	20	29	38
	Syndiesel, CO_2 [mill. t]	0	5	24	40	51	61	78	88
	MeOH chem., CO_2 [mill. t]	0,0	0,0	0,0	0,1	0,1	0,3	0,5	0,9
	BTX, CO_2 [mill. t]	0,0	0,1	1,1	3,7	8,0	14,0	26,2	52,9
	Olefins, CO_2 [mill. t]	0,00	0,13	1,15	3,70	7,71	13,23	24,37	48,35
	Urea, CO_2 [mill. t]	0	0,0	0,07	0,23	0,48	0,84	1,54	3,07
	Olefins, required MeOH [mill t]	0,00	0,10	0,83	2,69	5,61	9,63	17,74	35,21
Required biomass	MeOH, bio-based [mill. t]	0,00	0,08	0,25	0,62	1,15	1,86	3,44	5,47
	Bioethanol, fuel [mill. t]	89,37	93,93	96,10	98,25	94,57	84,18	72,49	59,38
	Olefins, bio-based; [mill. t]	0,00	4,22	8,75	13,63	18,88	24,54	38,30	53,20
	BTX, bio-based [mill. t]	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00

	Avoided CO2 incl. efficiency	2015	2020	2025	2030	2035	2040	2045	2050
Efficiency and steam	Chemicals [mill t]	0,0	0,2	1,4	4,6	9,7	16,7	30,9	71,4
	Fuels [mill t]	0,0	7,8	32,1	54,5	70,1	80,6	100,0	115,9
	Efficiency measures [mill t]	0,00	1,91	3,66	5,13	6,41	7,68	8,32	7,17
	Electricity based steam [mill t]	0,00	0,34	0,89	2,74	5,64	9,68	13,95	20,45
	Steam recompression [mill t]	0,00	0,03	0,08	0,27	0,59	1,02	1,48	2,18

Annex 5: Annual assumptions, impact and demand figures for the Max scenario

Pathways total		2015	2020	2025	2030	2035	2040	2045	2050
Production	MeOH via H_2, fuel [mill. t]	0	8	14	24	31	37	42	49
	Bioethanol, fuel [mill. t]	0,00	0,35	0,37	0,39	0,41	0,43	0,45	0,48
	Syn. Jetfuel [mill. t]	0,00	2,54	4,53	7,91	10,07	14,19	21,21	29,92
	Syndiesel [mill. t]	0	8	15	25	33	43	57	70
	MeOH via H_2 chem. [mill. t]	0,00	1,55	5,41	17,29	35,96	73,10	131,62	206,25
	Olefins via H_2 to MeOH [mill. t]	0,00	0,35	1,25	3,93	8,06	17,09	29,12	41,78
	BTX, via MeOH [mill. t]	0,00	0,17	0,58	1,89	3,97	7,70	14,79	25,28
	Ammonia via H_2 [mill. t]	0	0,2	0,6	1,8	5,1	9,7	14,8	19,8
	Urea via H_2 to NH_3; [mill. t]	0	0,1	0,3	1,0	2,8	5,3	8,1	10,9
	Chlorine [mill. t]	9,58	10,07	10,58	11,12	11,69	12,28	12,91	13,57
	MeOH, bio-based [mill. t]	0,00	0,00	0,01	0,02	0,05	0,07	0,18	0,31
	Olefins, bio-based [mill. t]	0,00	0,40	0,83	1,30	1,80	2,34	4,86	7,60
	BTX, bio-based [mill. t]	0	0	0	0	0	0	0	0
Avoided CO_2	MeOH, fuel [mill. t]	0,0	11,5	20,1	35,2	45,2	53,8	60,7	71,7
	Bioethanol, fuel [mill. t]	0,0	0,7	0,7	0,7	0,8	0,8	0,8	0,9
	Syn. Jetfuel [mill. t]	0,0	4,7	8,4	14,6	18,6	26,2	39,2	55,3
	Syndiesel [mill. t]	0,0	19,4	34,2	57,7	74,8	99,5	131,6	159,5
	MeOH via H_2, chem. [mill. t]	0,0	0,0	0,1	0,3	0,7	1,4	2,1	2,8
	Olefins via H_2 to MeOH [mill. t]	0,0	0,7	2,4	7,4	15,3	32,4	55,2	79,2
	BTX, via H_2 to MeOH [mill. t]	0,00	0,29	0,99	3,22	6,76	13,13	25,21	43,10
	NH_3 via H_2 [mill. t]	0,0	0,3	1,0	3,1	8,6	16,5	25,2	33,8
	Urea via H_2 to NH_3 [mill. t]	0,0	0,1	0,2	0,8	2,1	4,0	6,0	8,1
	MeOH, bio-based [mill. t]	0,00	0,00	0,01	0,03	0,05	0,09	0,21	0,37
	Olefins, bio-based; [mill. t]	0,00	0,99	2,05	3,19	4,42	5,75	11,97	18,70
	BTX, bio-based [mill. t]	not included							
Electricity demand	MeOH fuel [TWh]	0	91	159	279	358	426	480	568
	Syn. Jetfuel [TWh]	0	159	284	496	632	891	1331	1878
	Syndiesel [TWh]	0	532	938	1581	2048	2725	3605	4369
	MeOH chem. [TWh]	0,0	0,2	0,6	1,8	5,0	9,6	14,6	19,6
	BTX [TWh]	0,0	8,2	27,5	89,8	188,5	365,9	702,8	1201,6
	Olefins [TWh]	0	27	98	308	631	1337	2279	3270
	NH_3 [TWh]	0,0	2,1	7,3	23,1	63,4	121,5	185,3	248,5
	Chlorine [TWh]	45	42	41	40	40	39	38	38
	Steam generation [TWh]	0,0	2,0	5,2	16,3	33,9	59,0	87,1	134,7
	Steam recompr. [TWh]	0,0	0,0	0,1	0,2	0,3	0,6	0,9	1,3
	Carbon free electricity 2DS [TWh]	1670	2002	2337	2656	2920	3087	3254	3367
	% of carbon-free electricity (IEA2DS)	3%	43%	67%	107%	137%	194%	268%	348%
Required CO_2	MeOH as fuel, CO_2 [mill. t]	0	11	19	33	43	51	57	68
	Syn. Jetfuel, CO_2 [mill. t]	0	8	14	25	32	45	67	94
	Syndiesel, CO_2 [mill. t]	0	27	47	79	103	137	181	220
	MeOH chem., CO_2 [mill. t]	0,0	0,0	0,1	0,2	0,6	1,2	1,8	2,4
	BTX, CO_2 [mill. t]	0,0	1,0	3,4	11,2	23,5	45,6	87,6	149,7
	Olefins, CO_2 [mill. t]	0,00	1,09	3,93	12,33	25,28	53,60	91,36	131,09
	Urea, CO_2 [mill. t]	0	0,1	0,23	0,74	2,04	3,90	5,95	7,98
	Olefins, required MeOH [mill t]	0,00	0,79	2,86	8,98	18,41	39,03	66,53	95,45
Required biomass	MeOH, bio-based [mill. t]	0,00	0,12	0,42	0,99	1,82	2,90	7,08	12,57
	Bioethanol, fuel [mill. t]	89,37	93,93	96,10	98,25	94,57	84,18	72,49	59,38
	Olefins, bio-based; [mill. t]	0,00	4,22	8,75	13,63	18,88	24,54	51,07	79,80
	BTX, bio-based [mill. t]	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
Efficiency and steam	**Avoided CO2 incl. efficiency**	**2015**	**2020**	**2025**	**2030**	**2035**	**2040**	**2045**	**2050**
	Chemicals [mill t]	0,0	1,3	4,7	14,8	33,5	67,4	113,8	186,1
	Fuels [mill t]	0,0	36,3	63,4	108,3	139,4	180,3	232,3	287,5
	Efficiency measures [mill t]	0,00	1,83	3,47	4,56	4,53	3,84	2,97	2,15
	Electricity based steam [mill t]	0,00	0,34	0,89	2,74	5,62	9,61	13,80	20,20
	Steam recompression [mill t]	0,00	0,03	0,08	0,27	0,59	1,02	1,48	2,18

Annex 6: CO_2 capture technologies

Three main processes are imaginable to separate CO_2 effectively from flue gases: pre-combustion, post-combustion and oxyfuels capture. Every of the three processes requires different separation approaches because the treated gas mixture varies strongly. In pre-combustion the gas mixture consists mainly of H_2 and CO_2, in post-combustion the CO_2 is present together with N_2 and the oxyfuels process contains already near pure CO_2. The pre- and post-combustion capture is already widely applied and works by scrubbing of the flue gasses in special aqueous solutions.

Pre-Combustion

The gas mixture treated in the pre-combustion capture comes mostly from the gasification of coal or other higher hydrocarbons. It contains large amounts of CO_2 and H_2. The feed from the gasification is passed through a water-gas shift step to produce syngas. The remaining CO_2 is then separated.

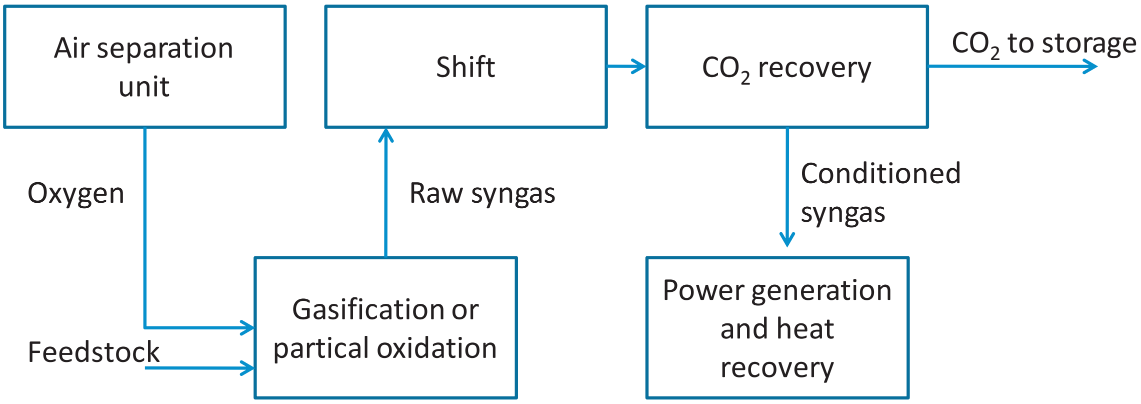

Figure 57: Post-Combustion capture scheme

Several processes for the separation of CO_2 from CO_2/H_2 gas mixtures are available at large scale. The most commonly applied technology for the capture of exhaust CO_2 is the amine washing, or amine stripping. Here the gasses are led through solutions of amines, where they react with the substances in the liquid. Subsequently the gasses are released (or stripped) from the rich solvent by pressure drop or heating. Typical amine solvents used are Monoethanolamine (MEA), Diethanolamine (DEA) or Methyldiethanolamine (MDEA). Alternatively, physical solvents such as refrigerated methanol, N-methyl-pyrrolidone or polyethylene glycol dimethyl ethers are used for physical absorption. These solvents are then stripped and the CO_2 is released by pressure drop or heating; which technique is applied depends on the solvent used.

Post-Combustion

Post combustion gas mixtures consist mainly of CO_2, N_2 and steam. These gas mixtures not only come from chemical plants but also from large scale power plants. From the different composition of pre- and post-combustion gases, the capture techniques vary but for both cases currently only absorption processes have been applied technically. Those will be described in the following section.

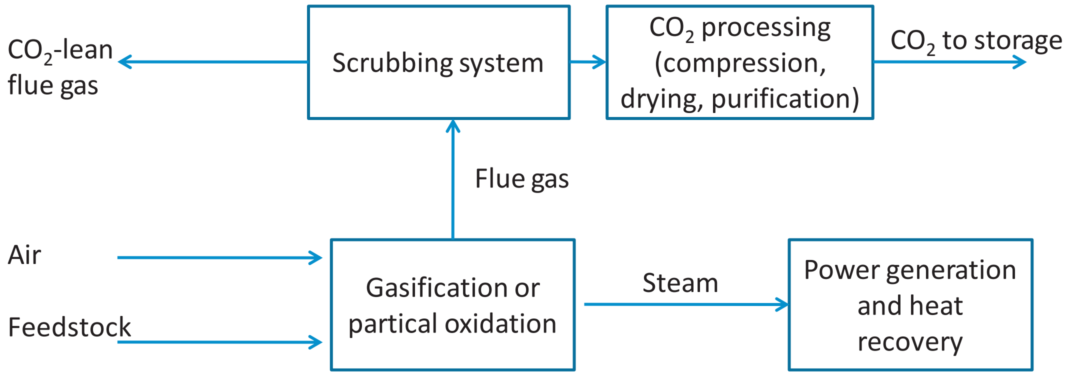

Figure 58: Post-combustion capture scheme

Amine scrubbing

The amine gas treatment with amine based organics (e.g. MEA or DEA, mono- or diethanolamine) is also called amine scrubbing and already industrially widely applied. The treated gas is led through a diluted amine solution at high pressures. From the enriched solution the solved gasses (CO_2 or H_2S) are later released by temperature increase or pressure drop. This stripping of the solutions to capture the CO_2 is very energy demanding and goes along with intense losses in pressure. This makes the CO_2 separation expensive and reduces the energy efficiency of power plants with carbon capture significantly.

Physical absorbents

In contrast to chemical washing fluids such as the described amines, the loading of physical absorbents increases with increasing pressure. High capture rates are therefore only realised at high CO_2-partial pressures, i.e. under pre-combustion conditions following gasification and CO-shift in a IGCC power plant. Common physical absorbents are refrigerated methanol, polyethylene glycol dimethylether or N-methyl-pyrrolidine.

Oxy-Fuels

The oxyfuels process has been proposed for the production of power and a simultaneous production of a flue gas stream that mostly contains CO_2 and H_2O. This exhaust stream would only need condensation of H_2O to form pure CO_2 for sequestration. The resulting energy penalty will presumably be much smaller than in the conventional power plants with CO_2 capture. Nevertheless, the technology needs purified O_2, which will be a drive to increase the cost above the conventional technologies.

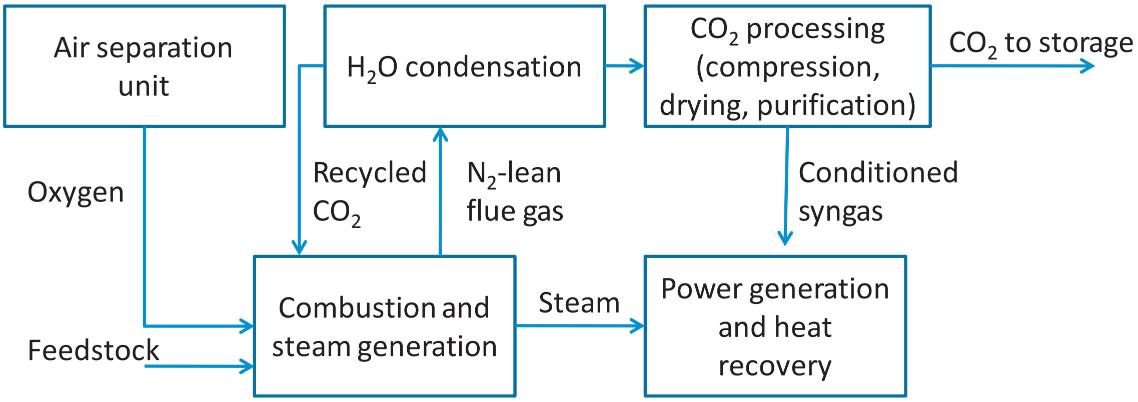

Figure 59: Oxy-Fuels Capture scheme

In order to reduce the energy penalty for the separation of CO_2 from exhaust gasses, new technologies will be needed and intense investigation actions have been undertaken over the last years. Especially membrane technology seems promising for a capture with little energy penalties. The TRL of these processes is mostly not above 4-5, and intense work needs to be done before these techniques can be applied in large scale. Especially the research on membranes from porous polymers and metal-organic frameworks has intensified in Europe, USA and Australia over the last years and the goal of 90% CO_2 at an energy penalty of less than 8% seams reachable in the coming years.

Direct air capture

Next to the capture of CO_2 from large scale factories, the direct capture from air should be addressed. Even though concepts are being discussed, none of those exceed a TRL of 2-3 for large scale capture. The low CO_2 concentration of only several 100 ppm in air provides a significant challenge for the direct capture of the gas from air.

The American Physical Society has done the following calculations, showing, that Direct Air Capture should be considered as the least favourable option in terms of plant footprint and energy requirement[131]:

A facility for capturing 1 $MtCO_2$/yr would require five structures, each 10 meters high and 1 km long, and could collect 1 $MtCO_2$/yr if air passed through at 2 m/s and 50% of the CO_2 were collected. The structures are spaced 250 meters apart, and the footprint of the system is roughly 1.5 km^2. Approximately six of these systems would be required to compensate for the emissions of a 1 GW coal plant.

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[131] Direct Air Capture of CO_2 with Chemicals - A Technology Assessment for the APS Panel on Public Affairs, APS 2011.

The theoretical minimum energy required to separate CO_2 from a gas mixture varies logarithmically, not linearly, with the CO_2 concentration. The thermodynamic minimum energy required to remove CO_2 from a mixture with an initial concentration of 0.04% (characteristic of air) is about three times larger than the corresponding minimum energy for an initial CO_2 concentration of 12% (characteristic of coal flue gas). The minimum values are 497 MJ/t CO_2 (21.86 kJ/mole) for 0.04% initial concentration and 172 MJ/t CO_2 (7.58 kJ/mole) for 12% initial concentration. This energy difference provides a reason why it is preferred to capture a large fraction of the CO_2 from concentrated point sources.

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