RENEWABLE CARBON INITIATIVE REPORT



CO₂ reduction potential of the chemical industry through CCU

A simplified exploratory scenario for CCU-based supply of embedded carbon for the global chemicals and derived materials sector

A paper of the Renewable Carbon Initiative, CO₂ Value Europe and nova-Institute

May 2022





The Renewable Carbon Initiative (RCI) is an interest group of more than 40 well-known companies founded in September 2020





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Imprint

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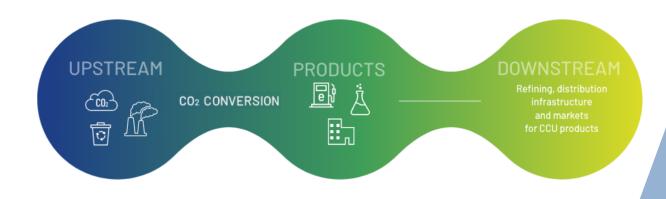
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WHO WE ARE

CO₂ Value Europe is the European association dedicated to Carbon Capture and Utilisation (CCU), bringing together stakeholders from the complete CCU value chain and across industries and sectors.



MISSION

 $\rm CO_2$ Value Europe's mission is to promote the development and market deployment of sustainable industrial solutions that convert $\rm CO_2$ into valuable products, in order to contribute to the net reduction of global $\rm CO_2$ emissions and to the diversification of the carbon feedstock to move away from fossil carbon.

VISION

Carbon Capture and Utilisation, also called Carbon Tech, is a broad term that covers all established processes that aim at capturing CO_2 – either from industrial point sources or directly from the air – and at converting it into a variety of products such as renewable fuels, chemicals and materials.

Our vision is a future where CCU has become an integral part of a low carbon economy, being of benefit to the climate, the economy and the people.

THE RENEWABLE CARBON INITIATIVE

Shape the Future of the Chemical and Material Industry

Renewable Carbon Initiative (RCI) was founded in September 2020. RCI members are committed to create a sustainable, fossil-free future for the chemical and material industry.

RENEWABLE CARBON INITIATIVE Elio-based CO₂-based Recycling

Circular Economy



WHY JOIN RCI?

RCI is an organization for all companies working in and on sustainable chemicals and materials – renewable chemicals, plastics, composites, fibres and other products can be produced either from biomass, directly via CO₂ utilisation, or recycling.

RCI members profit from a unique network of pioneers in the sustainable chemical industry.

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- Collective advocacy work to create a supportive regulatory and economic framework.
- Support in finding solutions for your specific problems on the way to your renewable carbon goals.

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Short version

Today, the production of chemicals and derived materials heavily relies on the use of fossil carbon. Industrial processes need hydrocarbons 1) to provide process energy (electricity and heat) for manifold processes and 2) to provide embedded carbon as feedstock for diverse substances, building-blocks, intermediates and derived materials such as polymers or detergents. Today, the embedded carbon accounts for approximately two thirds of greenhouse gas (GHG) emissions of most building blocks and intermediates of the chemical industry. To replace fossil carbon embedded in the chemical sector, renewable carbon sources are needed. These include:

- Renewable carbon gained from all types of biomass;
- Renewable carbon from captured **CO**₂ (CCU);
- Renewable carbon from recycling.

In an exploratory scenario, this study investigates the CO_2 emission reductions that can be achieved in the global chemical and derived material industries if the entire demand for embedded carbon is met solely and exclusively via CO_2 instead of from fossil sources.

In this study, methanol (CH₃OH) is considered to cover the needs for hydrocarbons for chemicals and derived materials. It is a plausible scenario to assign methanol a central role in supplying the chemical industry of the future. This is mainly for two reasons: Already today, methanol plays an important role in the chemical industry, being one of the most established commodities. In principle, a large proportion of organic drop-in chemicals can be produced from methanol through relatively short pathways¹. Secondly, methanol is the most direct efficient intermediate product made via hydrogenation of CO₂ with hydrogen. If you want to use CO₂ as a raw material for chemistry, producing methanol is the silver bullet, comparable to the production of ethanol from biotechnological pathways². Figure 1 shows the examined CCU-based pathway for methanol synthesis and the fossil-based reference process. The CCU-based production route includes CO_2 capture as a mix of direct air capture (DAC) and capture from point sources, hydrogen supply and the hydrogenation reaction for methanol synthesis. An electricity demand for these steps of 10,927 kWh per t of methanol is calculated.



¹ See Olah et al. (2018). While other chemicals produced from renewable sources may be more suitable for certain processes (e.g. e-hydrogen or e-methane), e-methanol is used as an exemplary production route for the future of the chemical and derived material sector.

² Another established option for the use of CO/CO₂ is through a biotechnological pathway towards the production of ethanol as a building block for the chemical industry. This study focuses on CCU-based methanol to explore possibilities of this specific scenario. Its only intention is to compare against fossil feedstock, assertions regarding other pathways based on renewable carbon cannot be derived.

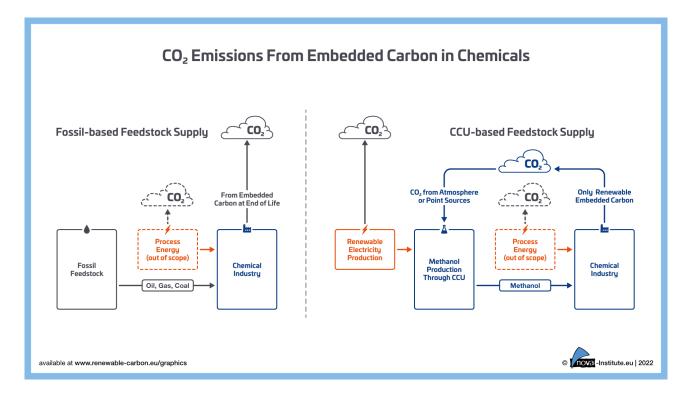


Figure 1: Current fossil reference in comparison to the examined CCU-based production of methanol for the chemical industry. The fossil-based, additional CO_2 emissions of the fossil reference system can be compared to the CO_2 emissions of the electricity production in the CCU system.

Replacing fossil feedstock with CCU-based methanol

In the scenario, fossil feedstock providing embedded carbon is replaced by CCU-based methanol (both measured in tons of carbon). Process energy is out of scope in both cases; also it can be expected, that the total energy demand for the downstream processes is higher for the fossil case.

In the fossil reference, the fossil-based embedded carbon contained in chemicals and materials is emitted to the atmosphere at their end of life, assuming complete oxidation (e.g. through combustion or (bio)degradation). In the CCU system CCU-based methanol replaces the fossil feedstock (based on the same amount of carbon). The corresponding electricity demand for methanol production causes CO_2 emissions (see below). But at the end of life, no additional carbon (or CO_2 , respectively) is emitted to the air because it was captured from the air (or from different point sources) before through carbon capture.

CCU is often an energy-intensive process, as CO_2 is an inert molecule and requires energy to be activated (chemically speaking: "reduced"). In order to avoid releasing more emissions through energy use than capturing via the CCU technology, energy supply for CCU has to be renewable. The GHG emissions related to CCU-based methanol synthesis depend on the emissions of the renewable energy production. The electricity mixes assumed for the calculation include average current emissions for photovoltaic as well as estimated emissions for renewable energy towards 2050. Emissions of CCU-based methanol could be 67 to 77 % lower compared to emissions from releasing embedded carbon of fossil fuels, when using current energy supply based on photovoltaics. With improvements in renewable energy production, the reduction could increase to levels between 96 and 100%, see Figure 2.



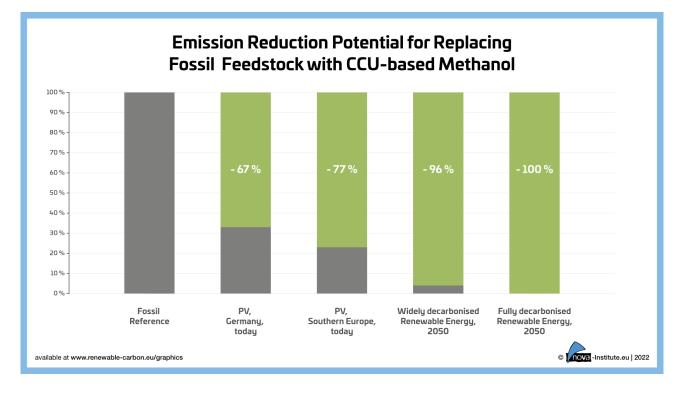


Figure 2: : CO_2 emissions derived from electricity supply for CCU used to produce methanol in comparison to the CO_2 caused by caused by complete oxidation of the carbon (fossil reference).

The specific GHG emission reduction potential per ton of methanol can be used to determine the total reduction potential if all fossil feedstock for the chemical industry was replaced by CCU-based methanol. The annual global demand for chemicals and derived materials can be estimated to rise to 1,000 million tonnes of carbon (Mt C) by 2050 (Kähler et al. 2021). Meeting this demand with CCU-based methanol would cause an immense demand of 29.1 PWh/year (29.1 x 10^{12} kWh) of renewable energy. Yet, with fully decarbonised energy supply, an amount of 3.7 Gt CO₂/year can be saved. These GHG emission savings are significant – even in comparison to today's global emissions of 55.6 Gt CO₂ eq/ year³. The result shows that CCU is a promising technology to reduce GHG emissions related to embedded carbon supply – if sufficient renewable energy is available. CCU-based carbon will be an important pillar of a future build on renewable carbon, complementing carbon from recycling and from biomass. To allow CCU to contribute to a climate-friendly supply of feedstock for the chemical industry global PV and wind capacities must be rapidly expanded.



³ Global annual GHG emissions, including land use change, according to PBL (2020)



CO₂ reduction potential of the chemical industry

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CO₂ reduction potential of the chemical industry through CCU

Long version

1. Introduction

Today, the production of chemicals and derived materials heavily relies on the use of fossil carbon. Industrial processes need hydrocarbons 1) to provide energy (electricity and heat) for manifold processes and 2) to provide embedded carbon as feedstock for diverse substances and products. Today, embedded carbon accounts for approximately two thirds of the carbon footprint (CO_2 emissions, which are released at end of life of a product) for most building blocks and intermediates, while emissions related to the production account for around one third, see Figure 3.

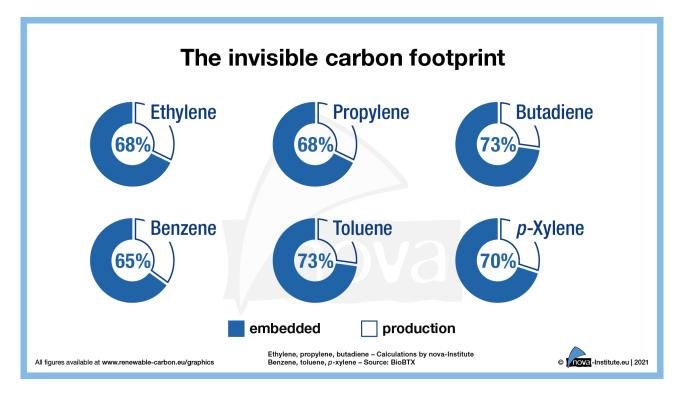


Figure 3: Carbon footprint of typical products from the chemical industry – shares of process energy and embedded carbon related CO₂ emissions.

Fossil fuels used for energy supply of the chemical sector can be replaced by renewable energies. This transformation is rightly referred to as "decarbonisation" of the energy sector, as carbonbased energy sources are replaced by alternatives that require no carbon. On the other hand, the chemical sector cannot be completely decarbonised because organic chemistry – by definition – relies on carbon since most products have carbon embedded in its molecules. Nonetheless, the use of fossil carbon must also here be phased out to mitigate climate change, a process referred to as



"defossilisation". This topic has so far received little attention⁴, but while emissions of the energy sector decrease through decarbonisation, the impact of embedded carbon becomes more and more relevant. If not targeted by appropriate measures, emissions from embedded fossil carbon will remain, even if other energy-related emissions decrease. To do so, renewable carbon sources must replace fossil feedstock for chemicals and derived materials. To replace fossil-based embedded carbon with renewable one, renewable carbon sources must be further deployed. These include:

- Renewable carbon gained from all types of **biomass**;
- Renewable carbon from captured **CO**₂ (CCU);
- Renewable carbon from **recycling**. (Carus et al. 2020)

Carbon Capture and Utilisation (CCU) stands for the capture and utilisation of carbon dioxide (CO_2) as a carbon source to be used as a feedstock in the production of synthetic fuels, carbonates, chemicals and polymers. (Carus et al. 2019)

While renewable carbon from biomass and recycling already contribute significantly to the supply of non-fossil carbon (biomass 10 % and recycling 5 %), the deployment of CO_2 utilisation is still comparatively small. Nonetheless, in the future it will play a substantial role in the supply of commodities with renewable carbon, intermediates such as methanol, ethanol, ethylene, propylene, naphtha or polymers such as PE, PP, PET or PUR. Hence, many studies investigate future opportunities for the use of CO_2 as a resource, see section 4. (Kähler et al. 2021)

The potential of CCU is practically unlimited, whereas the potential of biomass is limited due to e.g., land scarcity and biodiversity loss and recycling is only able to keep a certain share of carbon in the loop. Therefore, this paper investigates the climate change mitigation potential of CCU, if it were to deliver the entire carbon demand of the chemical and derived material industry.

In an exploratory scenario, this study investigates the CO_2 emission reductions that can be achieved in the global chemical and derived material industries if the entire demand for embedded carbon is met solely and exclusively via CO_2 instead of from fossil sources. For a highly simplified scenario, methanol is chosen as the most plausible pathway for the production of chemicals and materials from CO_2 . Thus, the simple scenario is used to explore the GHG saving potential of the use of CO_2 for chemicals and derived materials.



⁴ But this is changing, end of the year 2021, the term "defossilisation" has entered the political discussion, see for example: https://renewable-carbon-initiative.com/media/press/?id=304

2. Exploratory scenario for CCU-based methanol production

Today, the demand of the chemical industry is mainly met by cracking naphtha, which in turn is produced from crude oil. Other process routes start with natural gas/methane, fossil-based syngas or even methanol. With the bioeconomy, especially bioethanol and bio-naphtha are already available, CO_2 -based solutions as well as chemical recycling might represent additional sources for renewable naphtha, syngas and methanol in the near future. What will the raw material supply look like in 2050?

In this study, we focus on the embedded carbon in chemicals and plastics, which accounts for about two-thirds of the total carbon used in most chemicals today. The rest is used to supply the energy demand of chemical manufacturing (this process energy should also become renewable in future).

Methanol (CH₃OH) is considered to cover the needs for carbon for chemicals and derived materials. It is a plausible scenario to assign methanol a central role in supplying the chemical industry of the future. This is mainly for two reasons: Already today, methanol plays an important role in the

Excursus: Production capacity and applications for methanol

The global production capacity of methanol is expected to double in the eleven years from 2020 to 2030, from approximately 157 million metric tons in 2020, to around 311 million metric tons by 2030. This growth is attributable to approximately 131 planned and announced methanol plants, mainly located in the Former Soviet Union and Asia, that are expected to be operational between 2019 and 2030. (Fernández 2021)

The three major products made from methanol today are **formaldehyde** (36 %), **MTBE**¹/ **TAME**² (13 %), and **acetic acid** (9 %). Formaldehyde is, among others, used for the production of plastics and resins, pharmaceuticals, chemical fibres and paints and pesticides. MTBE/ TAME are mainly used as an octane booster in gasoline. The remaining 42 % are divided into the production of a large variety of chemical intermediates such as methyl terephthalate (DMT) for PET production, methyl methacrylate (MMA), chloromethane, methylamine and methanethiol, as well as the use of methanol and derivates as fuel in fuel cells or as diesel substitute (DME³). The plastic Polyoxymethylene (POM) is already mostly produced from methanol today (Bertau et al. 2014).

Furthermore, the condensation of methanol to produce hydrocarbons and even aromatic systems is the basis of several gas-to-liquids technologies. These include methanol-to-hydrocarbons (MtH), methanol to gasoline (MtG), methanol to olefins (MtO, ethylene/PE and propylene/PP). These conversions are catalysed by zeolites as heterogeneous catalysts.



¹ MTBE: Methyl tertiary-butyl ether

² TAME: Tert-Amyl methyl ether

³ DME: Dimethylether

chemical industry, being one of the most established commodities. In principle, a large proportion of organic drop-in chemicals can be produced from methanol through relatively short pathways⁵. Secondly, methanol is the most direct efficient intermediate product made via hydrogenation of CO_2 with hydrogen. If you want to use CO_2 as a raw material for chemistry, producing methanol is the silver bullet, comparable to the production of ethanol from biotechnological pathways⁶.

For a highly simplified scenario, the methanol scenario is therefore one of the most plausible. In the scenario, fossil feedstock used to provide embedded carbon is replaced by CCU-based methanol (both measured in tons of carbon). Process energy is out of scope in both cases. To assess the potential of the use of CO_2 , GHG emissions from the fossil feedstock, that occur at end of life of chemicals and derived materials, are compared to the GHG emissions from the necessary energy for the supply of CCU-based methanol. GHG emissions for the provision of the fossil feedstock are neglected (i.e., for extraction, extra transport, unintended methane emissions, etc.) but may lead to an even higher emission savings potential of CCU. An illustrative example is the production of petrol. Here, the extraction of fossil raw feedstock adds another 6.5 % to emissions from combustion at end of life, refining adds 9.5 %, transport and distribution add 2.5 %⁷. In the conservative estimation approach chosen here, emissions from extraction are neglected to the benefit of the fossil reference.

The scenario becomes an exploratory one when it is used to explore its implications such as future greenhouse gas emissions, which is the goal of this small study. In a first step, the methanol production route using CCU is examined. This includes carbon capture, hydrogen production and methanol formation. For these processes, current efficiencies are used to determine the electricity demand of one t of methanol.

For carbon capture, a mix of Direct Air Capture (DAC) and capture from point sources is assumed. For the production of hydrogen, current energy demand of Polymer Electrolyte Membrane (PEM) electrolysers is assumed. For the formation of methanol from CO_2 and hydrogen, the CO_2 hydrogenation reaction is assumed. In summary, the energy demand along the process chain is assumed as follows:

- CO₂ capture (DAC and point sources): 1,000 kWh/tco₂, see Table 2
- Hydrogen synthesis through Polymer Electrolyte Membrane (PEM) electrolysis: 50,000 kWh/t_H, (Birol 2019; Taibi et al. 2020)
- CO₂ hydrogenation with stoichiometric conversion⁸: 177 kWh/tco₂ (Pérez-Fortes and Tzimas 2016).

- 6 Another established option for the use of CO/CO₂ is through a biotechnological pathway towards the production of ethanol as a building block for the chemical industry. This study focuses on CCU-based methanol to explore possibilities of this specific scenario. Its only intention is to compare against fossil feedstock, assertions regarding other pathways based on renewable carbon cannot be derived.
- 7 According to the "most likely" scenario for EU conventional oil emissions estimates, see Brandt (2011)
- 8 Reactants are assumed to be completely converted to products. Hence, loss of reactants and corresponding burdens for recovery are neglected. Furthermore, possible distillation processes after the reaction to separate methanol from water are neglected.



⁵ See Olah et al. (2018). While other chemicals produced from renewable sources may be more suitable for certain processes (e.g. e-hydrogen or e-methane), e-methanol is used as an exemplary production route for the future of the chemical and derived material sector.

In a second step, grid emissions (in g CO_2 per kWh) of current and future renewable energy supplies are used to determine the GHG emissions caused by the production of one t of methanol. These emissions are compared to the end-of-life CO_2 emissions of equivalent fossil-based feedstock. Afterwards, the specific reduction potential using CCU-based methanol instead of its fossil counterparts is calculated.

Finally, the total GHG emissions are calculated, if all embedded carbon for organic chemicals and derived materials was replaced by CCU-based methanol. The results are then compared to findings of other studies and current GHG emissions of the industry sector.



3. Calculation of the energy demand for methanol production via CCU

Figure 4 shows the CCU production route of methanol considered in this paper and the electricity demand for the production of one t of methanol.

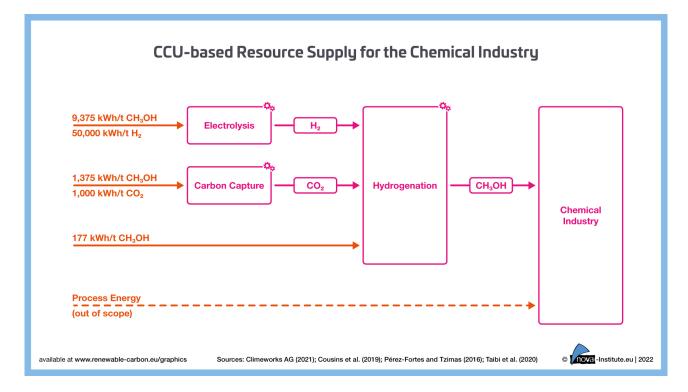


Figure 4: CCU-based process route for production of methanol (CH₃OH). Electricity demand is represented by red arrows. Below the arrow, the specific energy demand is stated, above, the contribution of the process to the total electricity demand of 1 t of methanol is stated. Assumptions for energy demand according to Climeworks AG (2021); Cousins et al. (2019); Pérez-Fortes and Tzimas (2016); Taibi et al. (2020). Purification and compression of hydrogen are neglected. For CO₂ hydrogenation, a complete reaction is assumed.

Beginning with the CO_2 hydrogenation – at the end of the production chain, methanol is synthesized in a catalytic, exothermic reaction. Table 1 shows the chemical equation and the mass balance for one ton of methanol per reactant and per element.

CO2	+	3H₂	→	СН₃ОН	+	H₂O
1,375 kg _{CO2}	+	187.5 kg _{H₂}	\rightarrow	1,000 kg _{CH₃OH}	+	562.5 kg _{H₂O}
	In: 187.5 kg 375 kg 1,000 kg	С		:	Out: 87.5 kg _{H₂} 375 kg _C ,000 kg _{O₂}	

Table 1: CO₂ hydrogenation reaction and mass balance of reactants

While the reaction is exothermic, energy input as well as an efficient catalyst are required⁹. The electricity demand for **hydrogenation of CO**₂ is:

177 kWh/t_{CH3OH} (Pérez-Fortes and Tzimas 2016). (1)

For **hydrogen** production using Polymer Electrolyte Membrane (PEM) electrolysis (η =84 %), the electricity demand is

50,000 kWh/t_H (Birol 2019; Taibi et al. 2020), (2)

or for one t of methanol, which requires 187.5 kg of hydrogen:

9,375 kWh/t_{CH3OH}. (3)

The **carbon** demand is covered by direct air capture (DAC) and from point sources. Table 2 provides an overview on energy demand of different technologies for CO_2 capture.



⁹ Due to its thermodynamic stability and kinetic inertness, energy and an efficient catalyst are needed to convert CO₂ into methanol. (Guil-López et al. 2019)

Table 2: Energy demand (heat and electricity) of various types of CO₂-capture, reported by different sources.

Source of CO ₂	Details	Reference	Energy demand per 1 t of CO_2		
			Heat	+ Electricity	= Total
Point source, pure CO ₂ ¹	Ammonia plant	(von der Assen et al. 2016)	0.01 GJ	0.4 GJ	114 kWh
Point source, pure CO ₂ ²	Bioethanol fermentation plants	(Müller et al. 2020)		0.432 GJ	120 kWh
Point source	Market pulp mills	(von der Assen et al. 2016)		1.03 GJ	286 kWh
Point source	Coal power plant	(von der Assen et al. 2016)		1.22 GJ	339 kWh
Point source	Gas power plant	(von der Assen et al. 2016)		1.6 GJ	444 kWh
Point source	Integrated pulp and paper mills	(von der Assen et al. 2016)	1.57 GJ	0.04 GJ	447 kWh
Point source	"H3" (Hitachi)	(IEA 2020)	2.4 GJ		667 kWh
Point source	"DC" (Shell Cansolv)	(IEA 2020)	2.5 GJ ³		694 kWh
Point source	"KS-1" (MHI), Sterically hindered	(IEA 2020)	2.6 GJ		722 kWh
Point source	"TS-1" (Toshiba)	(IEA 2020)	2.6 GJ		722 kWh
Point source	(Aker solution)	(IEA 2020)	2.8 GJ		778 kWh
Point source	"Ecoamine FG" (Fluor), Aqueous solution of MEA	(IEA 2020)	3.4 GJ ³		944 kWh
Point source	Cement	(von der Assen et al. 2016)	3.35 GJ	0.09 GJ	956 kWh
Direct air capture, future	Temperature-vacuum swing adsorption	(Deutz and Bardow 2021)	2.2 GJ ⁴	500 kWh	1111 kWh
Direct air capture		(von der Assen et al. 2016)	4.19 GJ	1.29 GJ	1522 kWh
Direct air capture	Temperature-vacuum swing adsorption	(Deutz and Bardow 2021)	4.7 GJ ⁴	700 kWh	2006 kWh

1 In this application, a stream of pure CO₂ is assumed. Energy demand only covers compression.



² In this application, a stream of pure CO₂ is assumed. Energy demand only covers drying and compression.

³ Calculated as average value of upper and lower value.

⁴ Heat pump used to produce low temperature heat from electricity (<100°C), stated value is the electricity demand (COP=2.51).

Not all currently available sources of CO_2 will remain relevant in the future. While CO_2 from power plants using fossil feedstock will be phased out, CO_2 emissions from cement production will likely remain available. Fermentation plants are lasting point sources, which can provide streams of nearly pure CO_2 . Existing fermentation plants are used in the food industry, biogas and bioethanol plants for energy. Further bioethanol production plants can be used to produce bio-based chemicals instead of using fossil feedstock. Furthermore, existing technology for gathering CO_2 from ambient air (Direct Air Capture, DAC) will be improved and likely be used widely. For these three CO_2 sources (bioethanol plants, cement production, and improved DAC), energy demands of 120, 956, and 1,111 kWh per t of CO_2 are reported, see Table 2. Considering this range, an average of 1,000 kWh/t CO_2 (3.6 GJ) is assumed for a mix of DAC and point sources, applying a conservative estimation. This corresponds in particular to the sources prospectively available in 2050.

The electric energy demand for carbon capture (covering electricity and heat) is:

$1,000 \text{ kWh/t}_{CO_{2}}(4)$

or for one t of methanol, which requires 1,375 kg of CO₂:

 $1,375 \text{ kWh/t}_{\text{CH}_{3}\text{OH}}$ (4)

All processes required to produce CCU-based methanol and the corresponding electricity demand are summarised in Table 3. The total electricity demand for the production of one t of methanol is 10,927 kWh. The electrolysis accounts for 86 % of the energy demand of the considered process chain.

Table 3: Production processes	for CCU-based methanol and	d corresponding electricity demand

Process	Specific energy demand
Carbon capture from DAC and point sources	1,375 kWh/t _{CH3OH}
H ₂ Electrolysis	9,375 kWh/t _{CH3OH}
CO ₂ hydrogenation	177 kWh/t _{CH3OH}
Total	10,927 kWh/t _{CH3OH}



4. Specific GHG reduction potential

The determined electricity demand of 10,927 kWh per t of methanol is used to determine the GHG emissions related to electricity production, considering different electricity sources. For comparison, a fossil reference scenario is included. The hereby compared pathways are displayed in Figure 5. In the fossil reference, the fossil-based embedded carbon contained in chemicals and materials is emitted to the atmosphere at their end of life, assuming complete oxidation (e.g. through combustion or (bio)degradation¹⁰). In the CCU system CCU-based methanol replaces the fossil feedstock (based on the same amount of carbon). The corresponding electricity demand for methanol production causes CO₂ emissions. At the end of life, no additional carbon (or CO₂, respectively) is emitted to the air because it was captured from the air (or from point sources) through carbon capture.

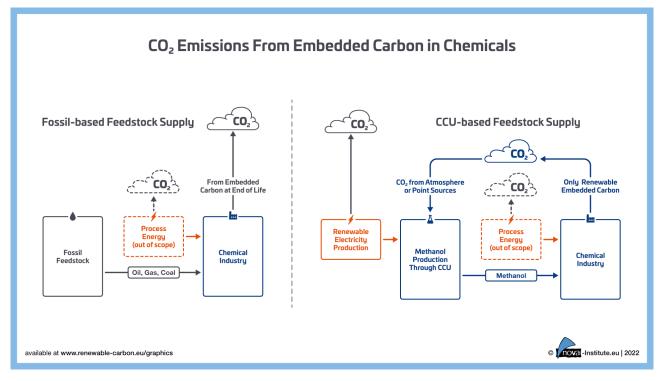


Figure 5: Current fossil reference in comparison to the examined CCU-based production of methanol for the chemical industry. The fossil-based, additional CO_2 emissions of the fossil reference system can be compared to the CO_2 emissions of the electricity production in the CCU system.

Table 4 shows the resulting GHG emissions related to electricity production needed to produce CCU-based methanol. The electricity mixes assumed for the calculation include current emissions for photovoltaic as well as estimated emissions for renewable energy towards 2050. With technology improvements and economies of scale, electricity efficiency and yield will increase and energy demand for the production will decrease (see e.g., Blanc and Marini (2014). Those



¹⁰ Carbon in some fossil products is emitted to the atmosphere directly when used, e.g. fuels, fuel additives or propellants. Other products emit fossil carbon to the atmosphere at the end of life, e.g. incineration of plastics. Again other fossil-based products have long lifetimes and therefore store carbon over longer periods (e.g. plastic furniture). Even if these long-lasting products are landfilled, the landfill gas occurring during degradation contains fossil carbon. Hence, assuming all fossil carbon ends up in the atmosphere is an appropriate simplification.

effects result in a decline of the carbon intensity (g CO_2 equivalent per kWh of electricity) in the future. With almost all input energy itself becoming renewable (including high-temperature heat and electricity), only few processes emitting CO_2 are left. An example of such a process is the reduction of SiO₂ using coal. The emissions related to electricity production with these assumptions can be estimated to be around 5 g/kWh ("Widely decarbonised renewable energy, 2050")¹¹. With ongoing decarbonisation of the energy sector and by replacing fossil carbon serving as a reduction agent with biochar or hydrogen, even direct emissions will disappear. Hence, even if enormously ambitious, future energy supply could become close to zero ("Fully decarbonised renewable energy, 2050")¹². Using a zero-emission assumption shows the final potential of the CCU technology. The CO₂ emissions related to electricity generation for CCU-based methanol can be compared to the CO₂ emissions at end of life of fossil feedstocks replaced by CCU-based methanol. Using 1 ton of methanol to replace fossil feedstock with the corresponding carbon content (375 kg C, see Table 1) saves 1,375 kg CO₂, which are not released as fossil CO₂ emissions at the end of life of the fossil feedstock. This comparison is shown in the last two columns of Table 4.

Table 4: CO₂ emissions caused by methanol synthesis for chemicals and derived materials for different renewable electricity mixes and comparison to CO₂ emissions at end of life of fossil feedstock for embedded carbon.

Process	Carbon intensity [g CO ₂ eq/ kWh]	Specific CO ₂ emissions [kg CO ₂ eq/ t _{CH3OH}]	CO ₂ emissions at end-of-life of equivalent fossil feedstock [kg CO ₂ eq/t _{CH3OH}]	CO ₂ reduction potential [kg CO ₂ eq reduction/ t _{CH3} он]
PV, Germany, today	42 ¹³	435		-922 (-67 %)
PV, Southern Europe, today	29 ¹³	317		-1,058 (-77 %)
Widely decarbonised renewable energy, 2050	511	1,375 52	-1,320 (-96 %)	
Fully decarbonised renewable energy, 2050	012	0		-1,375 (-100 %)

Depending on the assumptions for the carbon intensity of the electricity source, the reduction potential of replacing fossil feedstock with CCU-based methanol is between 67 and 100 %. These results are depicted in Figure 6.



¹¹ Estimation confirmed by Christian Breyer, Professor at Lappeenranta University of Technology, in personal communication on 21 September 2021.

¹² Zero emissions in the energy sector are also assumed by major publications, e.g. IEA (2021) or Ram et al. (2019). The renewable electricity supply uses a zero-emission assumption to show the potential of the CCU technology.

¹³ Currently, silicon wafer technologies are dominant in the Photovoltaic (PV) market, in particular multi c-Si. In an update of LCA studies for PV, Umweltbundesamt (2021) reports GHG emissions for electricity production from multi c-Si PV depending on the location of the PV modules of 36-47 g CO₂ eqkWh for Germany and 25-33 g for Southern Europe. In this study, average values are assumed for the reported bandwidths.

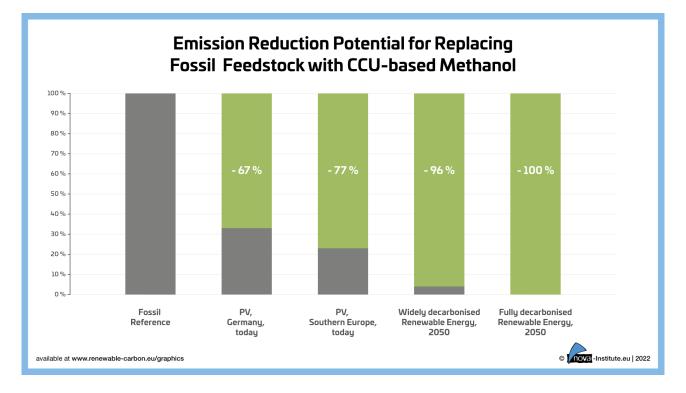


Figure 6: CO_2 emissions derived from electricity supply for CCU used to produce methanol in comparison to the CO_2 caused by complete oxidation of the carbon (fossil reference).

Using renewable energies, massive amounts of GHG emissions can be saved, if fossil fuel feedstock for chemicals and derived materials was replaced by hydrocarbons produced using CCU technology. Emissions from releasing embedded carbon in fossil fuels could be reduced by between 67 and 77 % using current renewable energy supply based on photovoltaics. With improvements in renewable energy production, the reduction potential could even increase to between 96 and 100 %.

Excursus: Excess heat from hydrogen electrolysis

For the production of hydrogen, large amounts of electricity are needed. Even though the efficiency is high (η =84% is assumed in this study), a share of energy will be converted to heat. Potentially, the excess heat can be used for industrial processes or district heating. The latter will become more relevant in the future, when combined fossil combined heat and power plants (CHP), which provide significantly to district heating today, are phased out. A study found, that high-temperature electrolysis has the potential to be fully integrated in industrial utility operations and heat utilization. For low-temperature electrolysis (like PEM electrolysis, assumed in this study), the use waste heat requires modern low-temperature direct heat networks. (Böhm et al. 2021)

Credits for heat use in CO₂ capture or in district heating are not considered in this study.



Table 5: Summary of other study's results in comparison to the findings of this study examining C. In some cases,the figures provided in the studies are converted to allow for comparison to this study. Blanks are left, if informationcannot be derived from provided data.

Source	CCU-based products in scope	Total electricity demand per unit of converted CO ₂ [kWh/t CO ₂]	Total electricity demand per unit of produced methanol [kWh/t _{CH3OH}]	GHG emissions per unit of methanol [kg CO ₂ / t _{CH3OH}]	CO ₂ reduction per unit of product [t CO ₂ reduction/ t product]
Kätelhön et al. (2019)	20 main chemical production routes	8,60214			
IEA (2019)	methanol		10,20015		
Artz et al. (2018)	methanol			500 – 1,000 ¹⁶	
Bhardwaj et al. (2021)	ethanol, methanol, jet fuels, etc.				2-11 ¹⁷
IRENA (2021)	methanol			10 – 650 ¹⁸	
DECHEMA (2019)	methanol		10,750		
Michailos et al. (2018	methanol		10,800	725 – 2,018 ¹⁹	
Ram et al. (2020)	methanol				1.8
This study (rounded)	methanol	8,000	10,900	0 – 450	0.9 – 1.4

14 In a "high-TRL" scenario, 32 PWh of electricity are required to convert 3.72 Gt of CO₂ and 0.59 Gt of hydrogen to methane and methanol.

- 15 In figure 22, page 43 of the report, a mature conversion technology pathway is examined, which uses 100 GWh of electricity to produce 54 GWh of methanol. Assuming an LHV of 19.9 MJ/kg_{CH3OH} methanol, this corresponds to 10,200 kWh/t_{CH3OH}.
- 16 In a best case scenario where the use of low-carbon energy and zero energy requirements for CO_2 capture and purification is assumed, GHG emissions are between 0.5 to 1.0 tonne CO_2 -eq / t_{CH_3OH} for both the direct and indirect conversion pathways. This corresponds to 74% to 93% reduction compared to the conventional production route.
- 17 In the study, 19 different CCU pathways (referred to as CO₂ recycling). Apart from chemicals, other sectors are included in the study with very large production volumes, e.g. fuels (ethanol, methanol, jet fuels, etc.). The large abatement potentials may be explained by focussing on highly processed chemical products (like jet fuels) instead of basic chemicals, such as methanol. Hence, the figures reported in this study represent other chemicals than methanol.
- 18 For e-methanol (from CO₂ and H₂) specific emissions of 0.5 to 33 g CO₂ eq per MJ methanol are reported, corresponding to 10 to 650 g CO₂ eq per kgmethanol with system boundaries from raw materials to final use, assuming a lower heating value (LHV) of 19.9 MJkg, see Table 11, p. 61 in the report.
- 19 In the LCA, system expansion is used to include a cement production plant, which serves as a point source for CO₂. For the production of 1 kg of methanol (and 1.96 kg of cement), GHG emissions are between 725 and 2,018 g CO₂ eqkgmethanol, depending on the electricity mix.



These results can be compared to outcomes of other studies. Table 5 summarises the comparison. It shows, that the majority of findings are of the same magnitude or even very close to the findings of this study. In particular the electricity demand per unit of produced methanol, a central metric, is in line with other studies. Larger GHG emissions in other studies are caused by either larger emissions per kWh of electricity or because the scope of the studies includes parts of processing to other chemicals/fuels. For example, largely higher CO_2 reductions per unit of product found by the study of Bhardwaj et al. (2021) may be due to the inclusion of highly processed chemical products (like jet fuels), which require much more energy in processing compared to the basic chemical methanol. In the case of the study by Michailos et al. (2018), system expansion is used to determine emissions from methanol production in combination with the production of cement, which is the source of the stream of CO_2 . Hence, the reported results are comparable only to a limited degree.



5. Total GHG reduction potential of the chemical industry using CCU

The specific GHG emission reduction potential per ton of methanol can be used to determine the total reduction potential if all fossil feedstock for the chemical industry was replaced by CCU-based methanol.

In a recent study published by nova-Institute, the amount of carbon contained in organic chemicals and derived materials²⁰ was determined. According to the study, the annual global demand for embedded carbon is 450 million tons (Mt) of carbon today and may rise to 1,000 Mt of embedded carbon by 2050. (Kähler et al. 2021)

In this study here, it is assumed, that the entire feedstock for these chemicals and derived materials is replaced by CCU-based methanol (including the feedstock, which is today met by biomass and recycling). One ton of methanol contains 375 kg of carbon (see Table 1). Hence, to replace fossil feedstock that contains one tonne of carbon, 2.67 t of methanol are required. To replace 1,000 Mt of carbon, 2,667 Mt of methanol are required. This would cause an immense demand of 29.1 PWh/ year (29.1 x 10¹² kWh) of renewable energy, which is approximately equal to today's global electricity production. Enormous efforts would have to be made to deploy sufficient renewable energy. However, if desert photovoltaic was used, around 117,000 km² of PV area would be needed to supply 29.1 PWh/year, which is only 0.7 % of the area of all subtropical deserts or 1.3 % of the Sahara²¹, see Figure 7. This large amount of electricity seems unrealistically high, but on second glance it becomes clear that there are no insurmountable technological limitations. It is definitely possible in the future.

With such a renewable energy supply, tremendous GHG emission reduction can be achieved: Assuming a zero-emission energy supply in 2050, the reduction potential is -1,375 kg CO_2/t_{CH_3OH} , see Table 4. Thus, replacing 1000 Mt of fossil carbon with CCU-based methanol can save 3.7 Gt of CO_2 emissions per year in 2050. Those savings are significant, even compared to the current global GHG emissions of 55.6 Gt of CO_2 eq/year²².



²⁰ Sectors included in the scope of the study are: Plastics, mainly thermoplastics, but also thermosets and elastomers or rubber; man-made fibres such as polyester; and organic chemical substances such as adhesives, solvents, detergents, paints, etc. Chemical products that don't contain any organic carbon are not included in the scope (e.g. nitrogen fertilisers and urea).

²¹ Assuming a desert PV-yield of 250 GWh/km² per year, 116,600 km² are needed to produce 29.1 PWh. Subtropical deserts have an area of 15.8 million km², the Sahara has an area of 9 million km².

²² Global annual GHG emissions, including land use change, according to PBL (2020)

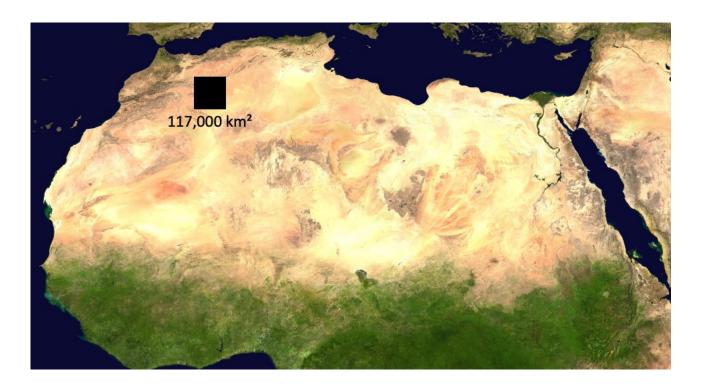


Figure 7: Photovoltaic area required for global CCU-based supply for chemicals and derived materials in relation to the Sahara (1.3 % of the Sahara area). Image source: NASA (2002, public domain)

6. Conclusion

In an exploratory scenario, this study investigates the CO_2 emission reductions that can be achieved in the global chemical industry and derived material industries if the entire demand for embedded carbon is met solely and exclusively from CO_2 instead of from fossil sources. In the scenario, the carbon demand of the chemical industry is completely covered by methanol from CCU. The replacement of fossil feedstock for embedded carbon with CCU-based methanol can reduce emissions by 67 to 77 % with current photovoltaic electricity supply and up to 96 to 100 % with clean renewable energy supply in the future. Even though the approach chosen for this study uses simplification, these results are generally in line with findings of many other studies. The amount of GHG emission savings of 3.7 Gt CO_2 /year is significant, even compared to the current global GHG emissions of 55.6 Gt of CO_2 eq/year²².

The result shows that CCU is a promising possibility to reduce GHG emissions related to embedded carbon supply, if sufficient renewable energy is available. To achieve the ambitious goals for climate mitigation, the chemical industry has to shift from fossil to renewable carbon sources. CCU-based carbon will be an important pillar of a future build on renewable carbon, complementing carbon from recycling and from biomass. To allow CCU to contribute to a climate-friendly supply of feedstock for the chemical industry global PV and wind capacities must be rapidly expanded.



7. References

Artz, J., Müller, T. E., Thenert, K., Kleinekorte, J., Meys, R., Sternberg, A., Bardow, A. and Leitner, W. 2018. Sustainable Conversion of Carbon Dioxide: An Integrated Review of Catalysis and Life Cycle Assessment. Chemical Reviews, Vol. 118 (2), 434-504. doi: 10.1021/acs.chemrev.7b00435

Bertau, M., Offermanns, H., Plass, L., Schmidt, F. and Wernicke, H.-J. 2014. Methanol: the basic chemical and energy feedstock of the future.

Bhardwaj, A., McCormick, C. and Friedmann, J. 2021. Opportunities and Limits of CO₂ Recycling in a Circular Carbon Economy: Techno-economics, Critical Infrastructure Needs, and Policy Priorities. Columbia | SIPA Center on Global Energy Policy (Ed.), Download at <u>https://www.energypolicy.columbia.edu/research/report/opportunities-and-limits-co2-recycling-circular-carbon-economy-techno-economics-critical</u>

Birol, F. 2019. The future of hydrogen: seizing today's opportunities. IRENA (Ed.), Download at <u>https://iea.blob.core.windows.net/assets/9e3a3493-b9a6-4b7d-b499-7ca48e357561/The_Future_of_Hydrogen.pdf</u>

Blanc, I. and Marini, C. 2014. Simplified prospective LCA models for residential PV installations based on SC-SI installed in Europe in 2050. Kyoto (Ed.), Download at <u>https://hal.inria.fr/hal-01115082/</u>

Böhm, H., Moser, S., Puschnigg, S. and Zauner, A. 2021. Power-to-hydrogen & district heating: Technology-based and infrastructure-oriented analysis of (future) sector coupling potentials. doi: 10.1016/j.ijhydene.2021.06.233

Brandt, A. R. 2011. Upstream greenhouse gas (GHG) emissions from Canadian oil sands as a feedstock for European refineries.

Carus, M., Dammer, L., Raschka, A., Skoczinski, P. and vom Berg, C. 2020. nova-Paper #12: "Renewable Carbon – Key to a Sustainable and Future-Oriented Chemical and Plastic Industry". nova-Institut (Ed.), Hürth, Germany, 2020-09. Download at <u>http://bio-based.eu/nova-papers/#novapaper12</u>

Carus, M., Skoczinski, P., Dammer, L., vom Berg, C., Raschka, A. and Breitmayer, E. 2019. Hitchhiker's Guide to Carbon Capture and Utilisation. nova paper #11 on bio- and CO₂-based economy. nova-Institut (Ed.), Hürth, Germany, 2019-02. Download at <u>http://bio-based.eu/nova-papers/#novapaper11</u>

Climeworks AG 2021. Articles and FAQ about direct air capture – How much energy is required to run Climeworks' direct air capture process?, Download at <u>https://climeworks.com/faq-about-direct-air-capture</u>



Cousins, A., Feron, P., Hayward, J., Jiang, K. and Zhai, R. 2019. Further Assessment of Emerging CO₂ Capture Technologies for the Power Sector and Their Potential to Reduce Cost. CSIRO report EP189975 (Ed.), Download at <u>https://ieaghg.org/ccs-resources/blog/new-ieaghg-technical-report-2019-09-further-assessment-of-emerging-co2-capture-technologies-for-the-power-sector-and-their-potential-to-reduce-costs</u>

DECHEMA 2019. Roadmap Chemie 2050. Auf dem Weg zu einer treibhausgasneutralen chemischen Industrie in Deutschland. DECHEMA and FutureCamp (Ed.), Frankfurt and Munich, Germany, Download at <u>https://www.vci.de/vci/downloads-vci/publikation/2019-10-09-studie-roadmapchemie-2050-treibhausgasneutralitaet.pdf</u>

Deutz, S. and Bardow, A. 2021. Life-cycle assessment of an industrial direct air capture process based on temperature–vacuum swing adsorption. Nature Energy, Vol. 6 (2), 203-213. doi: 10.1038/ s41560-020-00771-9

Fernández, L. 2021. Global production capacity of methanol 2018-2030., Download at <u>https://www.statista.com/statistics/1065891/global-methanol-production-capacity/</u>

Guil-López, R., Mota, N., Llorente, J., Millán, E., Pawelec, B., Fierro, J. L. G. and Navarro, R. 2019. Methanol synthesis from CO₂: a review of the latest developments in heterogeneous catalysis. Materials, Vol. 12 (23), 3902. doi: 10.3390/ma12233902

IEA 2019. Putting CO₂ to Use - Creating value from emissions. International Energy Agency (IEA) (Ed.), Download at <u>https://www.iea.org/reports/putting-co2-to-use</u>

IEA 2020. CCS on Waste to Energy. IEA (Ed.), Download at <u>https://www.club-co2.fr/</u>files/2021/01/2020-06-CCS-on-Waste-to-Energy.pdf

IEA 2021. Net Zero by 2050 - A Roadmap for the Global Energy Sector. International Energy Agency, (Ed.), Download at <u>https://www.iea.org/reports/net-zero-by-2050</u>

IRENA 2021. Innovation Outlook: Renewable Methanol. (Ed.), Download at <u>https://www.irena.org/</u>publications/2021/Jan/Innovation-Outlook-Renewable-Methanol

Kähler, F., Carus, M., Porc, O. and vom Berg, C. 2021. Turning off the Tap for Fossil Carbon – Future Prospects for a Global Chemical and Derived Material Sector Based on Renewable Carbon. nova-Institute (Ed.), Hürth, Germany, Download at <u>https://renewable-carbon.eu/publications/</u>product/turning-off-the-tap-for-fossil-carbon-future-prospects-for-a-global-chemical-and-derived-material-sector-based-on-renewable-carbon/

Kätelhön, A., Meys, R., Deutz, S., Suh, S. and Bardow, A. 2019. Climate change mitigation potential of carbon capture and utilization in the chemical industry. Proceedings of the National Academy of Sciences, Vol. 116 (23), 11187-11194. doi: 10.1073/pnas.1821029116

Michailos, S., Sanderson, P., Villa Zaragoza, A., McCord, S., Armstrong, K., Styring, P., Mason, F., Stokes, G., Williams, E. and Zimmermann, A. 2018. Methanol worked examples for the TEA and LCA guidelines for CO₂ utilization. doi: 10.3998/2027.42/145723



Müller, L. J., Kätelhön, A., Bringezu, S., McCoy, S., Suh, S., Edwards, R., Sick, V., Kaiser, S., Cuéllar-Franca, R. and El Khamlichi, A. 2020. The carbon footprint of the carbon feedstock CO₂. Energy & Environmental Science, Vol. 13 (9), 2979-2992. doi: 10.1039/D0EE01530J

Olah, G., Goeppert, A. and Prakash, G. 2018. Beyond Oil and Gas: The Methanol Economy . Wiley-VCH, Weinheim, Germany.

PBL 2020. Trends In Global CO₂ and Total Greenhouse Gas Emissions. PBL Netherlands Environmental Assessment Agency (Ed.), Download at <u>https://www.pbl.nl/sites/default/files/downloads/pbl-2020-trends-in-global-co2-and-total-greenhouse-gas-emissions-2019-report_4068.pdf</u>

Pérez-Fortes, M. and Tzimas, E. 2016. Techno-economic and environmental evaluation of CO_2 utilisation for fuel production. Synthesis of methanol and formic acid, doi: 10.2790/981669

Ram, M., Bogdanov, D., Aghahosseini, A., Oyewo, S., Gulagi, A., Child, M., Fell, H.-J. and Breyer, C. 2019. Global Energy System based on 100% Renewable Energy – Power, Heat, Transport and Desalination Sectors. (Ed.), 2019-03. Download at <u>http://energywatchgroup.org/wp-content/uploads/EWG_LUT_100RE_All_Sectors_Global_Report_2019.pdf</u>

Ram, M., Galimova, T., Bogdanov, D., Fasihi, M., Gulagi, A., Breyer, C., Micheli, M. and Crone, K. 2020. Powerfuels in a Renewable Energy World – Global Volumes, Costs and Trading 2030 to 2050. Deutsche Energie-Agentur (dena), Download at <u>https://www.dena.de/newsroom/publikationsdetailansicht/pub/study-powerfuels-in-a-renewable-energy-world-global-volumes-costs-and-trading-2030-to-2050/</u>

Taibi, E., Blanco, H., Miranda, R. and Carmo, M. 2020. Green Hydrogen Cost Reduction; Scaling up Electrolysers to meet the 1.5 C Climate Goal. (Ed.), Download at <u>https://www.irena.org/-/media/</u> <u>Files/IRENA/Agency/Publication/2020/Dec/IRENA_Green_hydrogen_cost_2020.pdf</u>

Umweltbundesamt 2021. Aktualisierung und Bewertung der Ökobilanzen von Windenergieund Photovoltaikanlagen unter Berücksichtigung aktueller Technologieentwicklungen. Umweltbundesamt (Ed.), Dessau, Germany, Download at <u>https://www.umweltbundesamt.de/sites/</u> <u>default/files/medien/5750/publikationen/2021-05-06_cc_35-2021_oekobilanzen_windenergie_photovoltaik.pdf</u>

von der Assen, N., Müller, L. J., Steingrube, A., Voll, P. and Bardow, A. 2016. Selecting CO₂ sources for CO₂ utilization by environmental-merit-order curves. Environmental science & technology, Vol. 50 (3), 1093-1101. doi: 10.1021/acs.est.5b03474

