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Environmental and Economic Performance of CO₂-Based Methanol Production Using Long-Distance Transport for H₂ in Combination with CO₂ Point Sources: A Case Study for Germany

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Abstract: The use of CO₂-based hydrocarbons plays a crucial role in reducing the climate footprint for several industry sectors, such as the chemical industry. Recent studies showed that regions which are favorable for the production of CO₂-based hydrocarbons from an energy perspective often do not provide concentrated point sources for CO₂, which leads to an increased environmental impact due to the higher energy demand of direct air capture processes. Thus, producing H₂ in regions with high renewable power potential and transporting it to industrialized regions with concentrated CO₂ point sources could provide favorable options for the whole process chain. The aim of this study is to analyze and compare pathways to produce CO₂-based methanol in Germany using a local CO₂ point source in combination with the import of H₂ per pipeline or per ship as well as H₂ produced in Germany. The environmental and economic performance of the pathways are assessed using life cycle assessment and cost analysis. As environmental indicators, the climate, material, water, and land footprints were calculated. The pathway that uses H₂ produced with electricity from offshore wind parks in Germany shows the least environmental impacts, whereas the import via pipeline shows the best results among the importing pathways. The production costs are the lowest for import via pipeline now and in the near future. Import via ship is only cost-efficient in the status quo if waste heat sources are available, but it could be more competitive in the future if more energy and cost-efficient options for regional H₂ distribution are available. It is shown that the climate mitigation effect is more cost-effective if the H₂ is produced domestically or imported via pipeline. Compared to the import of CO₂-based methanol, the analyzed H₂ import pathways show a comparable (pipeline) or worse environmental and economic performance (ship).

Keywords: CO₂-based methanol; H₂ import; environmental and economic assessment; defossilization



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1. Introduction

The dominant role of fossil resource use in the global energy and industry sectors continues to cause the major share of Green House Gases (GHG) emissions and a highly linear use of resources [1,2]. This strongly impels climate change in combination with a depletion of finite resources. Thus, the dismissal of fossil resource use is required to reduce GHG emissions and to use resources in a more circular way.

Two different concepts are discussed to end fossil resource use in industrial processes, namely decarbonization and defossilization. The former describes a reduction of carbon use in general and aims at processes where the carbon use can be substituted by different technologies, e.g., in the electricity sector [3,4]. The latter describes a substitution of fossil carbon sources with different carbon sources, such as CO₂ or biomass [5].

Hydrogen (H₂), produced with renewable electricity, is considered an important factor for decarbonization and defossilization strategies in multiple industry sectors. H₂ is produced via the electrolysis of water and represents an energy carrier that can be combusted without the emission of CO₂. Thereby, it offers options for long-term storage

and long-distance transport of volatile renewable electricity. Furthermore, it is required to substitute fossil resources in sectors where hydrocarbons cannot be directly substituted with electricity, e.g., in the chemical [6] or steel [7,8] industry. Thus, it is fundamental for climate-neutral energy and industry sectors, and a significant growth in the global H₂ demand from 90 Mt (2020) to 175 Mt (2030) up to 570 Mt (2050) is estimated within the coming decades [9]. Independent from the subsequent application, a low climate footprint of H₂ is a necessary premise to achieve climate benefits compared to fossil hydrocarbons [10]. Hence, regions with favorable conditions for renewable electricity generation are seen as promising locations for H₂ production and export [6]. However, the production and especially the transport of H₂ are still economically and technically challenging [11]. Further technological progress and cost reductions are necessary for H₂ value chains to become a viable alternative to fossil fuels.

For the chemical industry, which is responsible for more than 12% of global crude oil use and around 1 Gt of direct CO₂ emissions per year [12], neglecting fossil resources constitutes a challenge in two fields [13]. First, fossil-based heat and electricity production must be decarbonized using renewable energy sources. Second, fossil-based hydrocarbons must be substituted as carbon sources to produce organic chemicals. For the latter, a broad defossilization is necessary, which requires the exploration of new carbon sources [14]. Here, the use of CO₂ is considered an important step to abate fossil carbon sources via Carbon Dioxide Capture and Utilization (CCU) technologies [15]. The use of CO₂ opens up a broad field of possible synthesis pathways [16], while protecting biodiversity and the natural resources of land and water, whose use would be intensified in an unsustainable way if the chemical sector increases the use of biomass as a carbon source [17–19]. In addition, a recent study found that the application of CCU technologies could contribute to several other Sustainable Development Goals of the United Nations [20]. For the production of CO₂-based chemicals, the use of renewable electricity [21] or H₂ produced with renewable energy is elementary [22–24]. Therefore, the demand for H₂ by the global chemical industry, which is already the largest consumer, is expected to double from 70 Mt in 2020 to 140 Mt in 2050. In addition, the current H₂ sources, mainly natural gas, need to be substituted, which makes the chemical industry one of largest consumers for low-carbon H₂ now and in the future [6]. Furthermore, unavoidable CO₂ point sources or direct air capture should be used to source the necessary CO₂ to avoid lock-in effects and the delay of emission reductions [5]. From an economic perspective, CO₂-based chemicals are not yet competitive, but expected cost decreases in plant and energy costs could lead to a viable production in the near future [25,26]. At the same time, the use of CO₂-based chemicals in high-value markets could make their production viable already today without causing significant cost increases at the end of the value chain [27].

For the German chemical industry, which constitutes the largest chemical industry in Europe and the fourth largest in the world [28], this imposes specific opportunities and challenges. The use of CO₂ as a carbon source offers the chance to decrease the respective GHG emissions of more than 100 Mt CO₂-equivalents per year, especially in the field of scope 3 emissions, which account for about 50% of the total emissions. Furthermore, the current rate of secondary carbon input, which is below 1% [5], can be increased. Due to the high rate of industrialization in Germany, unavoidable CO₂ point sources will most likely continue to be available, offering sufficient amounts of CO₂ in comparably high concentrations [29]. However, the substitution of fossil carbon sources with CO₂ would require renewable energy in a quantity that corresponds to the current net production of electricity in Germany and most probably exceeds the future availability of renewable electricity [5,30,31]. Thus, the import of CO₂-based chemicals seems like a promising pathway, even though domestic production offers environmental and economic advantages [26].

Other options to counter this bottleneck for renewable energy are the construction of offshore wind parks owned or financed by specific industry sectors or the import of H₂ from regions with favorable conditions for renewable electricity production. Major chemical

companies in Germany currently pursue both options. The company BASF is constructing a 1.5 GW wind park in the North Sea together with Vattenfall. The company Covestro signed a long-term purchase agreement of 100 kt of H₂ per year that will be produced in Australia [32,33]. Furthermore, a consortium of several European grid operators for natural gas is planning to convert part of the current natural gas transportation and distribution pipelines into H₂ pipelines and combine them with new pipelines that also connect countries in Northern Africa to the European grid [34]. These options both enable the combination of local CO₂ sources with imported H₂ or offshore electricity production. Compared to the import of hydrocarbons, this offers a higher domestic value creation and supply security for carbon. In addition, CO₂ point sources are rare in regions favorable for renewable electricity production [26], wherefore the necessity to source CO₂ from the atmosphere is avoided, which significantly reduces the environmental impacts of CO₂-based chemical production.

However, the environmental impacts as well as the economic situation of H₂ production with electricity from offshore wind parks or its import to Germany in combination with a further use in chemical production have not been studied yet. Therefore, the research question of this article is the following: What are the environmental impacts and production costs related with the combination of imported H₂ and a CO₂ point sources in Germany, compared to the use of H₂ produced in Germany using electricity from offshore wind parks? As a case example, the production of CO₂-based methanol (MeOH) was chosen due to its broad application options as a base chemical.

This study extends the existing research by combining the analysis of spatially distributed H₂ production and transport with that of CCU technologies. The presented results allow a thorough characterization of CO₂-based methanol production using H₂ transported over a long distance from an environmental and economic perspective. The analysis has the following structure: (1) Description of the production systems and assessment methods. (2) Assessment of the environmental and economic performance using Life Cycle Assessment (LCA) and cost analysis. (3) Uncertainty assessment using Monte Carlo and sensitivity analysis.

2. Materials and Methods

2.1. Location Selection

The analysis of possible export countries for H₂ or hydrocarbons to the German or European market was part of several studies in the past [35–37]. The studies assessed the potential for renewable energy, which could be available for exports, economic aspects, technical aspects such as the availability of export infrastructure, as well as sociopolitical aspects such as the quality of bilateral relations or security. With respect to the necessary long-distance transport, three technologies are available, namely transport via *H₂ pipelines* and via ship using *Liquefied H₂ (LH₂)* or *Liquefied Organic Hydrogen Carriers (LOHC)* [38–40]. Each of the technologies offers specific advantages and disadvantages. On the one hand, transport via pipeline offers economic and environmental advantages compared to ship transport [39], but its construction requires a lead-time of several years and limits the available export options. On the other hand, import via ship is more flexible, with shorter lead-times, and it enables longer transport distances [37]. Furthermore, LH₂ is more costly than ship-transport via LOHC but causes less environmental impacts.

For the analysis in this article, Australia and Morocco were chosen as export countries. Both countries were identified as highly suitable for the import of H₂ to Germany in the studies listed above. Furthermore, the combination of both countries allows a thorough comparison between the import via Pipeline (Morocco) and ship using LH₂ and LOHC (both Australia) for the same use case. The exact locations for the H₂ production systems were derived from Gerhardt et al., (2020) [41] for Morocco and from the Australian Government (2021) [42] for Australia. They are located in Southern Morocco and Western Australia. Both regions offer comparably high-capacity factors for wind and photovoltaic (PV) plants, which enables high-occupancy rates for the electrolyzer using hybrid wind-PV plants for

electricity generation, which results in lower H₂ production costs [43]. In addition, Western Australia is geologically suitable to use salt caverns as a storage option between H₂ production and shipping [42]. Bremerhaven was chosen as the port of arrival in Germany. As transport distances, 2800 km (Morocco) and 18,000 km (Australia) were assumed. As input data for the capacity factors for the wind and PV plants, publicly available data from the global wind and solar atlas were used [44,45]. In general, the export from Morocco via ship would be possible as well; however, because of the environmental and economic advantages of the use of a pipeline [39], this option is not regarded in this article.

2.2. Environmental Assessment

The environmental impacts of the product systems were analyzed using LCA. The LCA study was carried out in accordance with international standards [46,47] and specific guidelines for the LCA of CO₂-based processes [29,48]. As functional unit, 1 kg of MeOH was considered. This base chemical is already used as feedstock for a variety of chemical or polymer products. Its importance is expected to further rise in the future, since it represents a promising option for the defossilization of the chemical sector [49]. Neither the chemical composition nor the use or end-of-life phase differ between fossil- and CO₂-based MeOH. Therefore, a cradle-to-gate analysis is sufficient in the context of this article. The environmental performance is analyzed by comparing the LCA results based on single impact categories. Like for the economic performance, a product system performs better if it shows lower values. The further calculation of an overall environmental performance that considers all impact categories in an aggregated manner was not part of this study. This would require the introduction of multi-criterial analysis, e.g., via the introduction of specific weighting systems, which would go beyond the scope of this study.

For the system modeling, the software openLCA was used in combination with the LCA database *ecoinvent* 3.5. Two types of uncertainty were regarded in the analysis. To include parameter uncertainty, specific parameter distribution derived from the available literature were regarded in the foreground system, and Monte Carlo Analysis (MCA) with 1000 runs was conducted for each product system. In addition, the uncertainty of the technical development of the product system is regarded with the help of a scenario analysis that considers improved technical parameters for the electrolyzer and expected structural changes (Table 1).

Table 1. Considered structural changes in the scenario analysis. ¹ Data for the grid mixes can be found in Supplementary Table S6.

System Element	2020	2030
Grid Mixes ¹	Based on actual data for grid composition in every country	Based on the national energy and climate action plans
Short Distance Transport	Via tube trailers or trucks	Via H ₂ pipeline distribution net
CO ₂ -Capture	Heat provision via fossil fuels	Heat provision via heat pumps

The climate footprint and three resource footprints were applied as indicators for the impact assessment. Recent studies showed that this set of indicators is an efficient and effective way to estimate environmental pressures in LCA with comparably few indicators, because the combination of these four footprints covers more than 84% of the possible environmental impacts of a product system [50]. Thereby, the climate footprint estimates the environmental pressures of GHG emissions, and the three resource footprints (Material, Water, Land) give information about the pressures of natural resource extraction [51–53]. As footprint indicators, the Raw Material Input (RMI) and Total Material Requirement (TMR) were used for the material footprint, the occupation of area for the land footprint, and the AWARE (Available Water Remaining) method for the water footprint. For the latter, only evaporation losses were considered, because water incorporation is not seen as problematic for CCU technologies [26], and the calculation of water dilution requires more detailed data than available.

2.3. Economic Assessment

To enable a thorough comparison between the results of the LCA and economic assessments, identical system boundaries for both analyses were considered [54]. For the economic assessment, the *Production Costs (PC)* and the *CO₂-Avoidance Costs (AC)* were calculated for the status quo, as well as for a 2030 scenario for each production pathway.

$$Production\ Costs_i = \frac{\sum_{t=1}^n \frac{Capex_t + Opex_t}{(1+WACC)^t}}{\sum_{t=1}^n \frac{Production\ Volume_t}{(1+WACC)^t}} \quad [€/t]$$

$$CO_2 - Avoidance\ Cost_i = \frac{Production\ Costs_i - Market\ Price_{fossil}}{GWI_i - GWI_{fossil}} \quad \left[\frac{€}{t\ CO_2eq.\ avoided} \right]$$

t: Period

i: Production Pathway

WACC: Weighted Average Costs of Capital

The PC are expressed as € per t produced chemical including the capital and operational costs for all required process steps. As capital costs, location-specific values were chosen based on an empirical analysis by Steffen (2020) [55]. The AC were calculated based on the PC and the results for the climate footprint. They indicate the respective costs to avoid the emission of one ton of CO₂-equivalents, i.e., the economic efficiency of climate mitigation measures. As costs for fossil MeOH, the average net market price of the last five years was considered in the status quo. For the future, a yearly price increase of 2% was considered according to the *stated policies* scenario published by the IEA [56].

As for the LCA, the uncertainties of the parameters and the system development were regarded in the economic assessment. For each cost parameter, a range was derived from the literature for the status quo and the future that results in a minimum, mean, and maximum value for the PC and AC. In the scenario analysis, structural changes were considered as well. A detailed list of the considered cost parameters and their values in the status quo and in 2030 can be found in the Supplementary Table S7.

2.4. System Description

The analyzed production systems consist of the process steps *electricity generation, water production and purification, H₂ production, H₂ transport (long distance), H₂ transport (short distance), CO₂ capture and MeOH synthesis* (Figure 1). If necessary, storage options were included as well. It was assumed that the CO₂ capture process and the MeOH synthesis would take place at a cement plant in the middle of Germany. For the MeOH production, the following five pathways were considered for H₂ provision:

- **Offshore:** H₂ production in Germany using electricity from an offshore wind park
- **Pipeline:** H₂ production and import via Pipeline from Morocco
- **LH₂:** H₂ production and import via ship from Australia
- **LOHC:** H₂ production and import via ship from Australia
- **LOHCwh:** H₂ production and import via ship from Australia using a waste heat (wh) source in Germany

In the following subchapters, the necessary processes are described in more detail. Further technical data and material balances can be found in Supplementary Tables S1–S5.

2.4.1. Renewable Electricity Production

To model the production of renewable electricity, data from UBA (2021) [57] was considered. The study contains actualized material and energy balances for offshore and onshore wind as well as PV plants. The material demand of the respective plants was adjusted to local conditions, i.e., the Full Load Hours (FLH) (Table 2). For electricity production in Australia and Morocco, a joint onshore wind and on-ground PV system was considered. For wind electricity, voltage (from high to low) and current transformation was

assumed, and the calculation of the combined FLH includes an overlap of 15% [58]. For Germany, an offshore wind plant in the northern sea was modeled 80 km from the coast. To model representative local conditions, an area of 100 km × 100 km within each region was considered, for which the mean FLH were calculated.

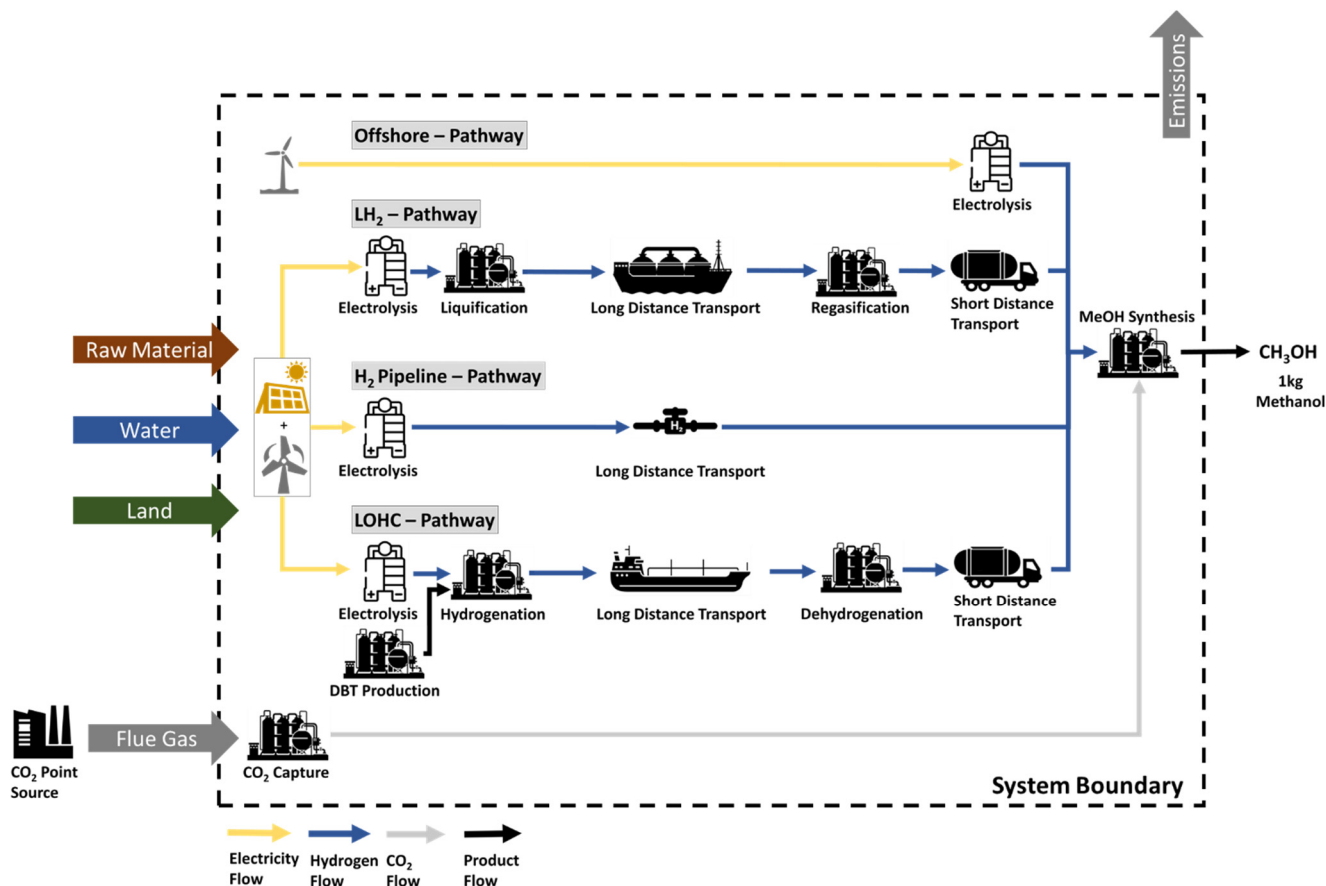


Figure 1. System description for the CO₂-based methanol production considering different production and import pathways for H₂. (DBT = Dibenzyltoluene, LH₂ = Liquefied Hydrogen; LOHC = Liquid Organic Hydrogen Carrier).

Table 2. Considered full load hours (FLH) for the local electricity production (PV = Photovoltaic).

Country	FLH Wind [h]	FLH PV [h]	FLH Combined [h]	Data Sources
Australia	3162	1861	4270	[44,45]
Germany	4745	–	4745	[45]
Morocco	5316	1900	6133	[44,45]

2.4.2. Water Production and Purification

According to Boulay et al. [59], the selected regions in Morocco and Australia suffer under water stress. To avoid additional pressure on the water availability in those regions, the provision of tap water via reverse seawater osmosis was assumed. Data for the process was taken from the ecoinvent database. As water input for the electrolyzer, a further purification of tap water is necessary. The purification step is modeled via a process from the ecoinvent database.

2.4.3. Water Electrolysis

To produce H₂, a Proton Exchange Membrane Electrolyzer system was modeled. In comparison to other electrolyzer types, such as Alkaline or High Temperature electrolyzer,

this system offers higher elasticities and shorter start-up periods [60], which makes it more suitable to use renewable energies with a volatile electricity generation. The material balances for the plant and the stack are taken from Bareiß et al., (2019) [10] and were specifically modeled according to the local conditions of renewable electricity production at every location. In the status quo, a system efficiency of 61% based on the lower heating value of H₂ is assumed. The operation takes place with a pressure of 30 bar and at 60 °C.

2.4.4. Pipeline Transport

For the transport of H₂ via pipeline, a hub-to-point concept was considered [40]. This assumes that the transmission pipeline and the demand location are directly connected without further distribution grids or lower pressure levels. As pipeline length, 2800 km were assumed, which would suffice to connect the assumed H₂ production location in southern Morocco with a cement plant in the middle of Germany following corridors of the existing pipeline grid for natural gas in Europe [41,61]. An amount of 25 km of this pipeline are assumed to be offshore, connecting Morocco with Spain. As the nominal operating pressure of the pipeline, 100 bar were assumed, with a pressure loss of 0.1 bar per km and a recompressing station every 500 km [34]. At every station, 0.5% of the transported H₂ is lost due to leakage [11]. The stations are assumed to be located in Morocco (1 Station), Spain (2 Stations), France (3 Stations), and Germany (1 Station), and each is operated with the local grid mix.

The pipeline was modeled according to concepts for H₂ pipelines presented in the literature. It has a diameter of 1000 mm, a wall thickness of 2.3 cm, and is built with conventional X70 Steel, which is considered suitable for H₂ pipelines [62,63]. To model the pipeline in OpenLCA, the existing processes for on- and offshore transmission pipeline construction in the ecoinvent database were modified accordingly. In addition, the pipelines are assumed to be coated with a tin coating to reduce H₂ diffusion [40,64]. A steel demand of 557 kg/m and a coating demand of 109 kg/m were assumed. In total, the modeled pipeline would have a H₂ transmission capacity of 77 TWh/a. A lifetime of 40 years was assumed [65].

2.4.5. Liquefied H₂ (LH₂)

To transport H₂ as fluid, several process steps are needed after the production step. At first, the H₂ is stored in a salt cavern to allow a decoupling of H₂ production and ship loading. To model its storage in a salt cavern, data from Wulf et al., (2018) [64] were used. As input pressure, 85 bar are assumed, and as output pressure, 50 bar are assumed. Prior to the long-distance transport of H₂, it needs to be liquefied to raise the energy density. For the liquefaction process, a H₂ input stream at 20 °C and 20 bar is cooled, then pressurized and expanded to reach a temperature of −250 °C and a pressure of 2 bar [66,67]. An initial compression is necessary due to the negative Joule Thompson coefficient of H₂, which leads to a cooling of the gas while being compressed until reaching a temperature of −71 °C. After reaching this temperature, an expansion is necessary for further cooling.

For the long-distance transport, a modified tanker for Liquefied Natural Gas with a transport capacity of 140,000 m³ H₂ was considered [68]. During the transport, H₂ losses occur due to imperfect tank insulation. The liquefied H₂ warms up and switches to the gas phase, which raises the pressure in the tanks. The emerged gaseous H₂ gets released and can be used as a substitute for ship fuel [69]. These kinds of H₂ losses are described as boil-off losses. In this article, a boil-off loss of 0.216% per day was assumed. Together with a travel distance of 18,000 km (port to port) from Geraldton to Bremerhaven according to Seadistance.org [65], in combination with a speed of 12 knots, this leads to 34 days of travel time and thus 7.2% of H₂ losses per transport. To model the ship transport, an existing process in the ecoinvent database was modified. For every transport, two routes, one loaded and one unloaded, were considered.

After the transport, the H₂ is regasified, i.e., heated up using the ambient temperature [11]. The short-distance transport is assumed to happen on the road using tube trailers at

500 bar pressure [39,70]. The trailer was modeled according to existing examples, and the material balances can be found in the Supplementary Table S5. As mean transport distance, 400 km were assumed. The different transport capacities between long- and short-distance transport also require an additional storage step, wherefore the storage in a salt cavern in northern Germany was assumed.

2.4.6. LOHC

The transport of H₂ using LOHC requires a H₂ carrier as well as a hydrogenation step at the starting location and a dehydrogenation step at the final destination. As a carrier, dibenzyltoluene (DBT) was considered in this study, because it offers comparably high-energy densities combined with low levels of flammability and toxicity, and low production costs [71]. The material balance for its production was derived from Wulf and Zapp (2018) [39]. In the hydrogenation step, the DBT is loaded with H₂ in an exothermal reaction using platinum and aluminum as catalysts. Per kg DBT, 62 g of H₂ can be stored corresponding to 6.2%wt. Before and after the loading, the LOHC is stored in chemical tanks at ambient pressure.

It is assumed that the ship transport happens with common oil tankers with a transport capacity of 150,000 t at a speed of 12 knots, resulting in 34 days of traveling time. To model the transport via ship, an existing process in ecoinvent was adjusted according to the respective transport volume, travel speed and transport distance [72]. For each trip, two transports were considered, one with loaded LOHC and one with unloaded LOHC. The exchange of loaded with unloaded LOHC takes place at each port, wherefore two sets of LOHC and chemical storage tanks are required. Potential H₂ losses were derived from an average value for losses occurring during crude-oil transport of 0.2% [73]. The short-distance transport to the MeOH plant is modeled via an ordinary oil truck with a mean distance of 400 km.

The endothermic dehydrogenation step takes place at the MeOH plant and requires temperatures above 300 °C [39]. It is assumed that the necessary heat is either supplied by burning part of the transported H₂ or by a waste heat (wh) source. For the former, around 27% of the hitherto transported H₂ is necessary [71,74], and the dehydrogenation step would cause significant losses of H₂. After the dehydrogenation, the H₂ needs to be compressed from ambient pressure to 30 bar, which is the same output pressure as for the electrolysis step. The required electricity for the compressors is provided by the German grid mix.

2.4.7. CO₂ Capture and MeOH Synthesis

To model the CO₂ capture process, the capture from a cement kiln in combination with heat integration from a MeOH synthesis reactor according to Meunier et al., (2020) [75] was considered.

For the MeOH synthesis, an operating pressure of 80 bar was assumed, which makes further compressing steps necessary for the CO₂ input flow as well as for the H₂ input flows for the offshore and LOHC pathways. The pipeline and LH₂ pathways deliver the H₂ at around 100 bar or 500 bar, respectively, and no additional compression is necessary. The required electricity for the compressors is provided by the German grid mix. As material input, 1.42 kg_{CO₂} and 0.197 kg_{H₂} are required per kg MeOH [23,76]. For the scale of the plant, 100 kt_{MeOH} per year were assumed, which corresponds to the largest CO₂-based MeOH plant being built at the moment [77]. For the fossil-based MeOH production, a process for the German market from the ecoinvent database was used as a reference process.

3. Results

3.1. Energy Balances

The results for the energy balances for the production of 1 kg_{MeOH} show how much energy is directly required for each pathway and how much of it is lost in the production and transport processes (Figure 2). For the methanol, a lower heating value of 21 MJ/kg

was assumed. The balances are further differentiated in energy efficiency values, i.e., how much of the energy input is lost within the product system, and how much H₂ is lost due to dissipation or its use in transformation processes.

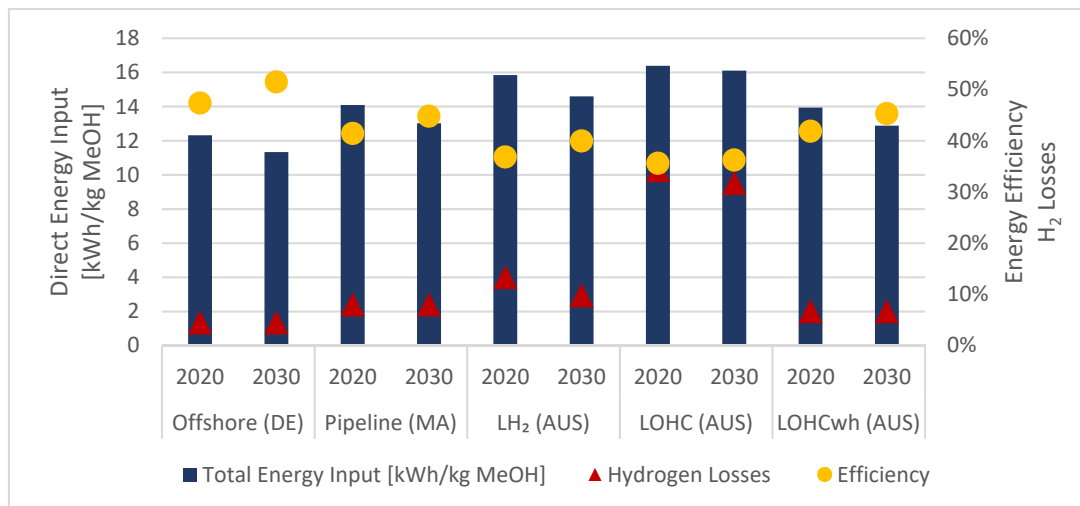


Figure 2. Required direct energy input, energy efficiency, and process-related H₂ losses for the different H₂ provision pathways for the production of 1 kg CO₂-based MeOH in Germany. H₂ losses happen through dissipation or utilization as energy sources in the transformation processes. (AUS = Australia, DE = Germany, FR = Fossil Reference, MA = Morocco, LH₂ = Liquefied Hydrogen, LOHC = Liquid Organic Hydrogen Carrier, Offshore = H₂ production with electricity from an offshore wind park, wh = waste heat usage).

In general, at least half of the direct energy input is lost within the considered pathways in the status quo. The offshore pathway shows the lowest overall energy demand, the highest energy efficiency, and the least H₂ losses per kg CO₂-based MeOH. Here, H₂ losses only occur in the MeOH synthesis step, and no transportation is required. If imported H₂ is used, 14 (pipeline) to 33% (LOHC) more energy is required to produce the same product. Compared to the import via pipeline, the studied shipping pathways require more energy input and cause higher H₂ losses due to the necessary transformation processes or the transport. Only if a source for waste heat is available, this pathway shows comparable values to the import via pipeline. For the future, efficiency gains between 1 to 5% can be expected, mainly due to increased process efficiencies for the electrolyzer and the transformation processes, as well as fewer compressing steps for the short distance transport.

3.2. LCA Results

3.2.1. Environmental Footprints

The results for the environmental footprints show a trade-off between the different impact categories (Figure 3). On the one hand, all processes show lower climate footprints than the fossil reference with H₂ production in Germany and with the import via pipeline clearly outperforming the import via ship. Furthermore, for all environmental footprints, the import pathways cause higher impacts than for the offshore pathway, with the pipeline route being the best import alternative in every category and the LH₂ pathway outperforming both LOHC pathways. On the other hand, the CO₂-based MeOH production generally causes higher environmental impacts for all other footprints. The only exception is the water footprint for the offshore pathway; here, less evaporation losses occur than for the fossil-based production. In addition, the RMI of the offshore pathway is about the same as for the fossil-based production. The assumed structural changes in 2030 lead to generally lower environmental impacts, especially for the importing pathways. This is mainly caused by the more carbon-extensive grid mixes and more energy-efficient options for the short

distance transport, which make the transport less impactful. Nevertheless, the existing trade-offs would not be avoided.

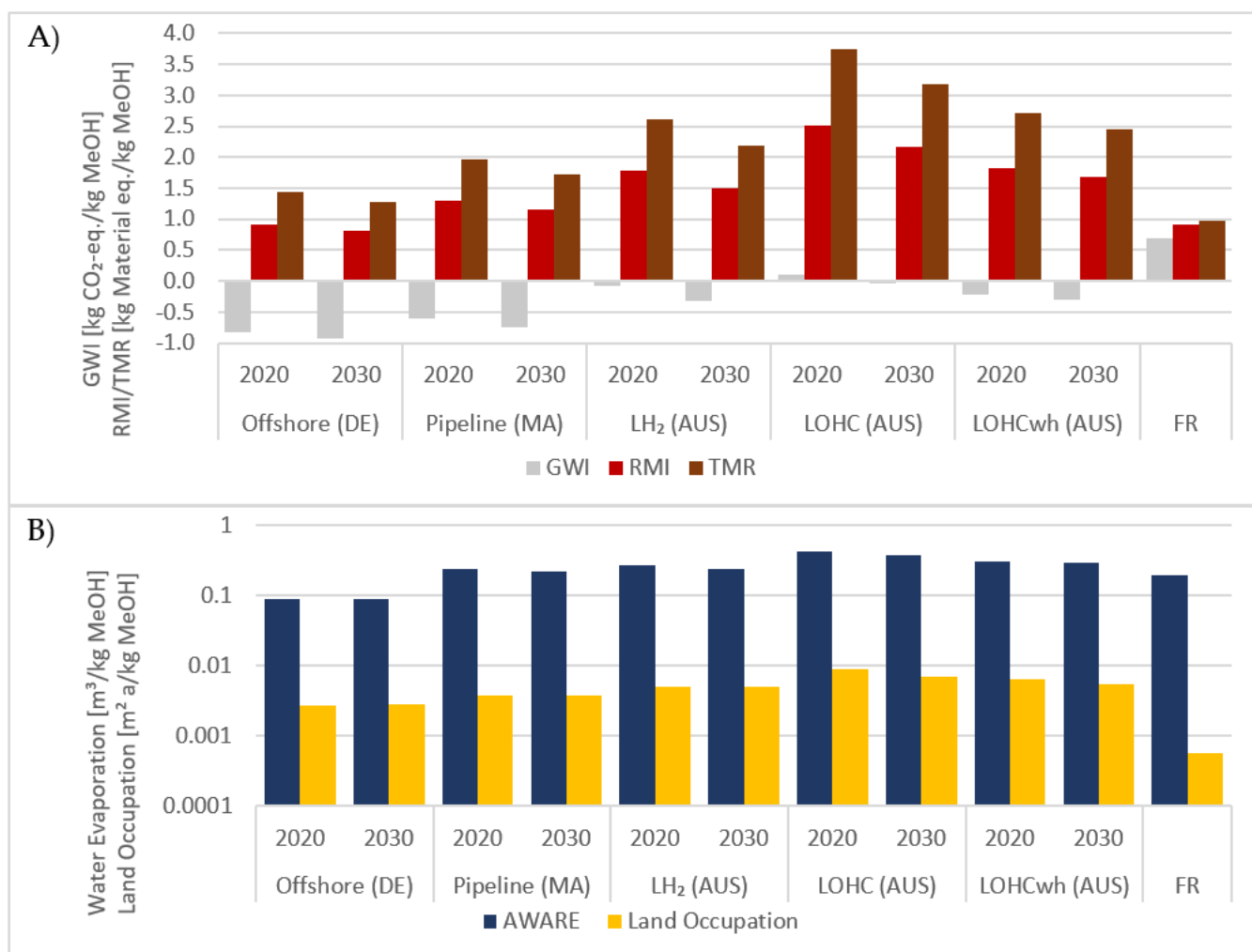


Figure 3. Results of (A) the climate and material as well as (B) the water and land footprint for fossil (FR) and CO₂-based MeOH production in 2020 and in 2030, based on different production pathways for H₂. For the fossil reference, no substantial deviations can be expected for the future, wherefore only the values for the status quo were considered. (AUS = Australia, DE = Germany, FR = Fossil Reference, MA = Morocco, LH₂ = Liquefied Hydrogen, LOHC = Liquid Organic Hydrogen Carrier, Offshore = H₂ production with electricity from an offshore wind park, wh = waste heat usage; GWI = Global Warming Impact; RMI = Raw Material Input; TMR = Total Material Input; AWARE = Available Water Remaining).

3.2.2. Process Contribution to Footprints

The results of the contribution analysis show the major drivers of the environmental impacts as well as the higher complexity of the import pathways (Figure 4). In general, H₂ production and transport are the dominating factors. For the climate and especially for the material footprint, the electrolysis step, i.e., the production of the required electricity, contributes the major part of the footprints (GWI: 31–45%; RMI: 48–69%). The impact of the electrolysis step increases proportionally with the H₂ losses within the pathways, wherefore this impact is generally higher for the import via ship. The more transformation and transport processes are required, i.e., the more complex the product system is, the higher the environmental impacts. In most cases, the electricity demand for compression steps is responsible for large shares of the impacts. Especially for the import pathways via ship, the multiple transformation and storage steps cause pressure losses that require

additional and energy-intensive recompressing. This was also shown by the results for the energy balances. For the hydrogenation and dehydrogenation steps of the LOHC pathways, the necessary platinum catalyst also significantly raises the material and climate footprint as well as the production of the required DBT as the carrier material. The short distance transport only matters for the import via the LH₂ pathways, due of the pressure of 500 bars required for the transport in tube trailers. For the pipeline pathway, the contribution of the pipeline construction is below 3% of the total impacts and thus plays a minor role compared to the impacts of the pipeline operation. The impacts of CO₂ capture and MeOH synthesis are mainly caused by the German grid mix for heat and electricity.

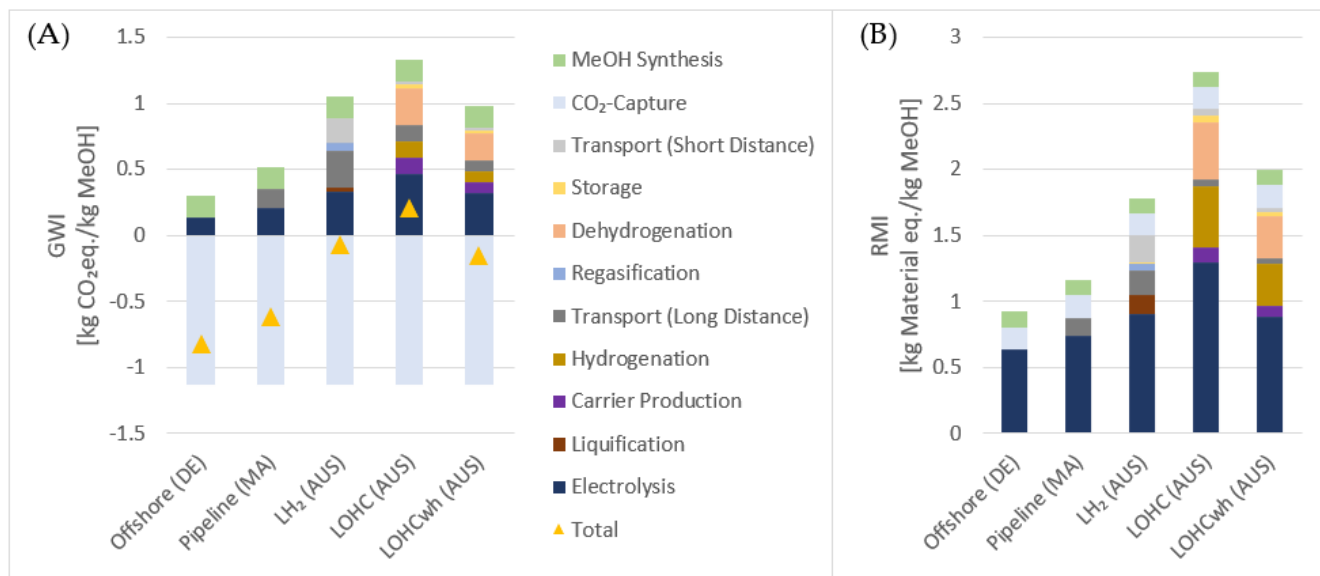


Figure 4. Process contributions to (A) the climate and (B) the material footprint for all considered MeOH production pathways. The legend refers to both graphs. (AUS = Australia, DE = Germany, MA = Morocco, LH₂ = Liquefied Hydrogen, LOHC = Liquid Organic Hydrogen Carrier, wh = waste heat usage; Offshore = H₂ production with electricity from an offshore wind park; GWI = Global Warming Impact; RMI = Raw Material Input).

The results also show how sensitive the product systems are towards the environmental footprints of electricity provision, even though the electrolysis is assumed to be fully provided with renewable electricity. It is important to note that if the Australian grid mix is used for the local storage and transformation processes, the environmental impacts in general and specifically the climate footprint increase significantly. The climate footprint of the Australian grid of 0.97 kg_{CO₂-eq.}/kWh would cause GWI values of 1.4 kg_{CO₂-eq.}/kg_{MeOH} (LH₂) or 0.4 kg_{CO₂-eq.}/kg_{MeOH} (LOHC), i.e., an increase by a factor of 20 (LH₂) or 4 (LOHC). Whereas for the LOHC pathway, the climate footprint remains lower, this would cause a higher climate footprint than for fossil-based MeOH production for the LH₂ pathway. Furthermore, for the import via pipeline the climate footprint would be raised by 17% if the first compression step is provided by the Moroccan grid mix. Thus, the energy providers for the auxiliary processes have an important impact and need to be carefully examined in practice.

3.2.3. Parameter Distribution

The result distributions of the MCA show a difference between the pathways and enable a comparison between the impact of parameter uncertainty and technology selection (Figure 5, Supplementary Figure S1 and Table S8). If the standard deviations of the different production pathways are compared, the import via ship shows higher values, i.e., a higher uncertainty, than the import via pipeline or the offshore pathway. At the same time, the ranking of the pathways does not change if parameter uncertainty is considered. For

all pathways, more than 75% of the results are lower than the next worse alternative. Consequently, the parameter variation has a lower impact on the results than the selection of the technology to provide H₂ for the MeOH synthesis. In the case of the climate footprint, the worst-case values for all pathways except LOHC are still lower than the climate footprint of the fossil alternative. For the LOHC pathway, few outliers provide higher values. At the same time, even in the best case, a trade-off between climate footprint reduction and an increase in the material footprint cannot be avoided for the import pathways. In contrast, for the offshore pathway, it is avoided in around 25% of the cases.

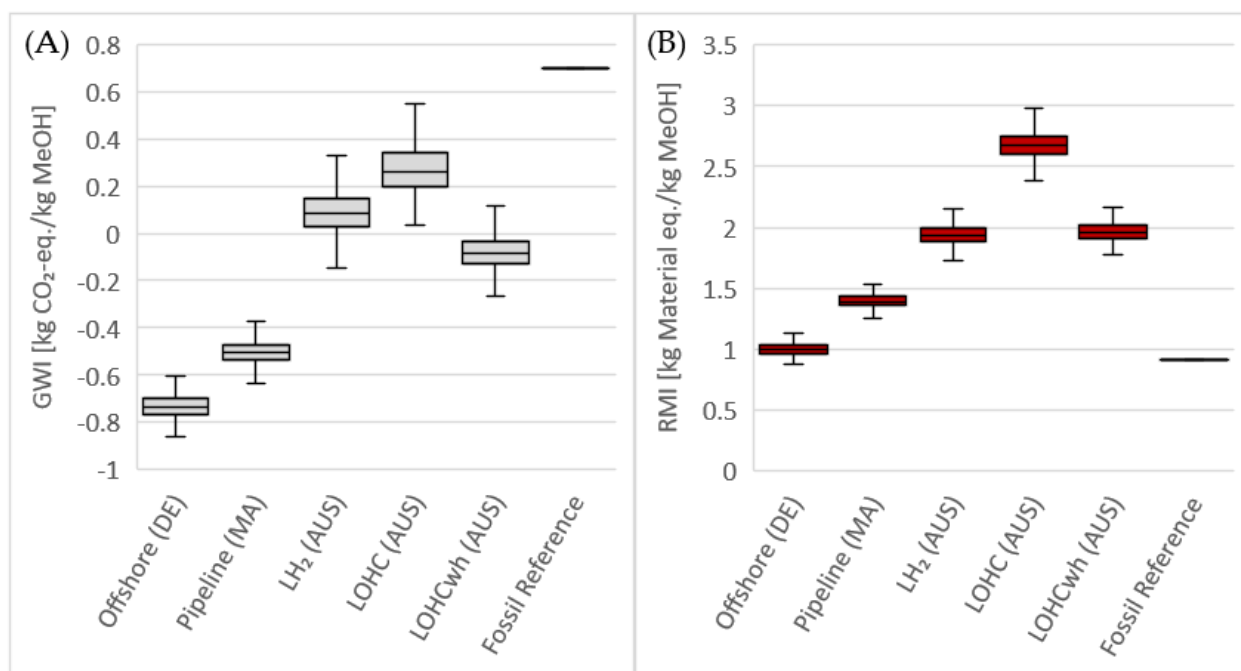


Figure 5. Box plots showing the uncertainty distribution of (A) the climate and (B) the material footprint for all considered MeOH production pathways. Outliers are not shown for graphical reasons. (AUS = Australia, DE = Germany, FR = Fossil Reference, MA = Morocco, LH₂ = Liquefied Hydrogen, LOHC = Liquid Organic Hydrogen Carrier, wh = waste heat usage; Offshore = H₂ production with electricity from offshore wind park; GWI = Global Warming Impact, RMI = Raw Material Input).

3.3. Economic Results

3.3.1. Production Costs

The results for the production costs show a different picture than for the environmental impacts (Figure 6). Economic competitiveness compared to fossil-based MeOH can be reached neither now nor in the near future. In addition, the regarded import pathways via pipeline or LOHCwh are more promising than the offshore pathway. Furthermore, the differences in between the pathways are lower for the production costs than for the environmental impacts. The alternative with the lowest production costs in 2020 is the H₂ transport via pipeline (1333 €/t_{MeOH}). Ship transport only shows lower costs than the offshore pathway (1616 €/t_{MeOH}) if waste heat is available. The import of LH₂ is the most expensive pathway in the status quo, mainly due to the costs for short-distance transport, which are dominated by the investment costs for the tube trailer (20% of the total costs). For the offshore pathway and the import via pipeline, the electrolysis step is a more decisive cost driver (70–84% of the total costs) than for the import via ship. Beside the lower technical complexity of these pathways, this is also caused by higher electricity costs (Germany) or higher capital costs (Morocco) than in Australia. For the import via ship, the H₂ transport causes 14% (LOHCwh), 28% (LOHC), or 43% (LH₂) of the total costs. Thus, competitive advantages in lower H₂ production costs are partly or completely compensated. The CO₂ capture and MeOH synthesis together cause between 14 (LH₂) and 22% (LOHCwh) of the

total costs. The cost ranges show that the production costs could be 20% lower in the best case, but also 30% higher in the worst case. In addition, the results of a sensitivity analysis further illustrate the high influence of the electrolysis step for all pathways, but also its reduced impact for the import via ship (Supplementary Figures S2 and S3).

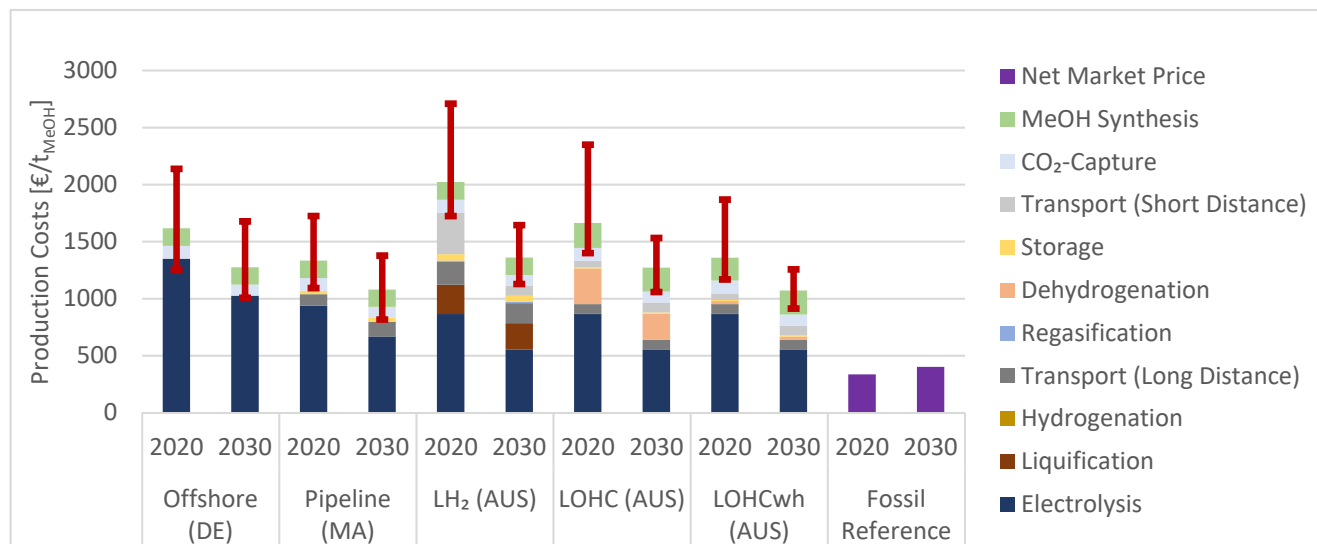


Figure 6. Production costs for CO₂-based MeOH, including cost ranges. The values for 2030 represent nominal values, i.e., no adjustment for a future inflation rate is conducted. (AUS = Australia, DE = Germany, FR = Fossil Reference, MA = Morocco, LH₂ = Liquefied Hydrogen, LOHC = Liquid Organic Hydrogen Carrier, Offshore = H₂ production with electricity from offshore wind park, wh = waste heat usage).

In 2030, reduced electricity and plant costs as well as more energy-efficient short distance transport could lead to a reduction of production costs between 19% (Pipeline) and 33% (LH₂). Nevertheless, the cost ranking of the alternatives does not change. Despite the relatively higher cost reduction for the import pathways via ship, the LH₂ and LOHC pathways still show higher costs than the offshore pathway. Due to the parameter uncertainty, no clear best alternative can be identified among the import pathways via ship without waste heat sources and the offshore pathway, because they all show similar value ranges. At the same time, the minimum and maximum values for the pipeline and LOHCwh pathways are clearly lower than for the other alternatives. Thus, in the status quo and the future, the LH₂ and LOHC pathways are not competitive towards the offshore pathway either from an economic or from an environmental perspective.

The mean costs for H₂ provision at the MeOH plant range from 5.2 (Pipeline) up to 8.9 €/kg_{H₂} (LH₂) in the status quo and 4.2 (Pipeline) to 5.6 €/kg_{H₂} (LH₂) in 2030. To achieve competitive MeOH production under the assumed circumstances, H₂ provision cost below 0.4 (status quo) and 0.7 €/kg_{H₂} (2030) would be necessary.

3.3.2. CO₂-Avoidance Costs

If the climate footprint and the production costs are regarded in combination, it becomes clear that the import via ship shows significantly higher AC than the offshore and pipeline pathways now and, in the future, (Figure 7). In the status quo, the minimum avoidance costs are above 500 €/t_{CO₂-avoided} but could be reduced to 330 (Pipeline) or 412 €/t_{CO₂-avoided} (Offshore) in the future. Thus, the climate mitigation effect for the offshore or pipeline pathway is and remains more cost-efficient than for the import via ship.

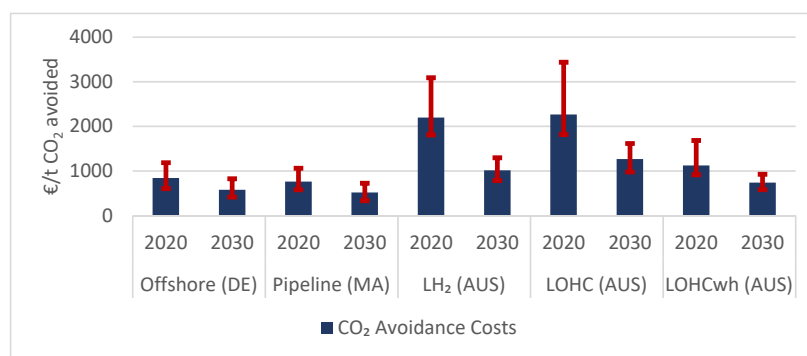


Figure 7. CO₂ avoidance costs of the different CO₂-based methanol production pathways considering ranges for the production costs, assuming substitution of fossil-based methanol. (AUS = Australia, DE = Germany, FR = Fossil Reference, MA = Morocco, LH₂ = Liquefied Hydrogen, LOHC = Liquid Organic Hydrogen Carrier, Offshore = H₂ production with electricity from an offshore wind park, wh = waste heat usage).

In general, the AC for MeOH production strongly depends on the costs and the climate footprint of the provided H₂ (Figure 8). In the status quo, avoidance costs below 100 € /tCO₂-avoided are only possible for H₂ provision costs below 1 €/kgH₂ in combination with a climate footprint below 2 kgCO₂-eq./kg kgH₂. At the same time, a climate footprint above 9 kgCO₂-eq./kgH₂ would lead to higher climate footprint for the CO₂-based production. The pathways analyzed in this article show a GWI of 1.8 (offshore) to 5.4 (LOHC) kgCO₂-eq./kgH₂. In the 2030 scenario, AC of 100 € are possible for H₂ provision costs up to 1.5 €/kg H₂ in combination with a climate footprint up to 2 kg CO₂-eq. per kgH₂ (Supplementary Figure S4).

		Hydrogen Provision Costs [€/kg H ₂]										
		0.4	1	2	3	4	5	6	7	8	9	10
GWI [kg CO ₂ -eq./kg H ₂]	0	0	77	195	314	433	552	670	789	908	1027	1145
	1	0	87	222	356	491	626	761	896	1030	1165	1300
	2	0	101	256	412	568	723	879	1035	1191	1346	1502
	3	0	119	304	488	672	857	1041	1226	1410	1595	1779
	4	0	146	372	598	825	1051	1277	1503	1729	1956	2182
	5	0	189	481	773	1066	1358	1650	1943	2235	2527	2820
	6	0	267	680	1093	1506	1919	2332	2745	3158	3571	3985
	7	0	454	1158	1862	2566	3270	3974	4677	5381	6085	6789
	8	1	1534	3911	6288	8665	11,042	13,419	15,795	18,172	20,549	22,926
	9	IE	IE	IE	IE	IE	IE	IE	IE	IE	IE	IE

Figure 8. CO₂-avoidance costs for CO₂-based methanol production in Germany, depending on the production costs and climate footprint of the used H₂. (GWI = Global Warming Impact, IE = Increase in Emissions).

4. Discussion

The German chemical industry needs sources for non-fossil carbon in combination with large amounts of renewable energy to defossilize the production of organic chemicals. Due to probable scarcities of sufficient renewable energy capacities in Germany, alternative pathways for the provision of renewable energy need to be considered. In this article, the production of CO₂-based MeOH using unavoidable CO₂ point sources in Germany in combination with imported H₂ was analyzed for the first time. The import of H₂ via pipeline or ship was compared with H₂ production in Germany using offshore wind as an energy source and assessed environmentally and economically. The climate footprint of MeOH production can be reduced in every case, but the results show several trade-offs between the environmental impact categories as well as between the environmental and economic results. Though the offshore pathway shows the least environmental impacts, it is comparably expensive at the same time. Furthermore, the reduction of the climate footprint would lead to an increased use of other resources in almost every case. Among the import pathways, the import via pipeline is the most promising. An import via ship seems only

reasonable if sources for waste heat or local H₂ pipeline grids for short-distance transport within Germany are available. The following in brief compares the results of this article to the existing literature and discusses the implications for practice and future research.

The analysis in the article for the first time combines the production and transport of H₂ with CO₂-based chemical production. For that reason, the results of this article need to be compared to the existing literature in both fields. Several studies analyzed the production and the transport of H₂ from an environmental or economic perspective. Those studies mostly focused on the mere production and provision of H₂ without a specific use case, its short distance distribution [38,71], or its use in the transport sector, as well as for energy storage [11,39]. Transport via pipeline was identified as the alternative with the least environmental impacts [64] and costs [71]. Furthermore, Wulf and Zapp (2018) [39] also described the trade-off between environmental impacts and economic performance for transport via LH₂ and LOHC. The authors calculated climate footprints between 1.5 (Pipeline) and 5.8 kg_{CO₂-eq.}/kg_{H₂} (LOHC), which are similar to the results of this article (1.8 to 5.4 kg_{CO₂-eq.}/kg_{H₂}). The differences are caused through different assumptions for the transport distance and the electricity providers. Heuser et al., (2019) [38] described the influence of transformation and transport processes on the import costs for LH₂. They calculated costs of 4.4 €/kg_{H₂}, which differ from the results of this study for the status quo, because lower costs for electricity, a shorter transport distance, and no regional distribution after the ship transport were regarded. For the 2030 scenario, the results are identical. Hank et al. [78] calculated H₂ provision costs for the import from Morocco to Germany via ship of 4.2 (LH₂) and 5.1 €/kg_{H₂} (LOHC). The differences compared to the results of this study can be explained by lower assumed electricity and capital costs, as well as a shorter transport distance and the exclusion cost-intensive short-distance transport. Thus, the core results for H₂ production and transport of this study are comparable with previous studies and complement the existing literature with a detailed and combined environmental and economic assessment of a concrete use case for imported H₂ in the chemical industry.

With respect to the MeOH production, the results of this study differ slightly from previous studies. For example, in case of the climate footprint, either lower [21] or higher values [22] were hitherto calculated, with the results of this study lying in the existing range. The deviations can be explained by different assumptions for the electricity and CO₂ source. With respect to trade-offs between environmental impact categories and the risk of problem-shifting by importing CO₂-based energy carriers or chemicals, a similar overall situation can be found in the literature [22,26,79].

Compared to the import options analyzed in this article, the import options for CO₂-based MeOH analyzed by Kaiser et al., (2021) [26] offer a higher energy efficiency due to simpler and more efficient transport processes, which also reduces the environmental impacts. Regions with favorable wind conditions exhibit a better performance than all studied pathways using imported H₂. Furthermore, the combination of local CO₂ point sources with imported H₂ shows a better or comparable performance for the pipeline pathway than MeOH imported from PV-based locations, especially if direct air capture is used as a CO₂ source. In contrast, the import via ship without the availability of waste heat shows higher environmental impacts than all analyzed production locations for CO₂-based MeOH, including those using direct air capture as a CO₂ source. For the 2030 scenario, the situation does not significantly change. With respect to the economic situation, the costs for most of the locations for the import of CO₂-based MeOH are lower in the status quo (933–1666 €/t_{MeOH}) and in 2030 (588–889 €/t_{MeOH}) compared to the calculated values for the production based on imported H₂ in this article (2020: 1254–2709 €/t_{MeOH}; 2030: 817–1645 €/t_{MeOH}). Thus, the import of CO₂-based MeOH would probably allow lower market prices and lower CO₂ avoidance costs. However, the use of imported H₂ would enable a higher domestic value creation, because two main process steps (CO₂ capture and MeOH synthesis) would take place in the importing country. In addition, the use of local sources could increase the independency from global markets and therefore lower supply risks for carbon. Nevertheless, to achieve a competitive advantage, the costs

for H₂ transport (long- and short-distance) need to decrease significantly. This could happen through process optimization and scale-up, as well as the integration of H₂ transport pathways in the existing industrial infrastructure by using redesignated pipelines and potential sources for waste heat.

Compared to the fossil-based production of MeOH, several approaches should be pursued to achieve economic competitiveness. First, the investment costs for all involved technologies need to be reduced significantly. Second, CO₂-based chemicals should be used as input to produce high-value polymer products. This would allow a cost covering production without causing significant increases in production costs [27]. Third, the externalities of fossil carbon use as material should be consequently internalized, e.g., by the introduction of input quotas for non-fossil carbon sources. These approaches require expenditures for research and development, the overtaking of investment risks by companies, as well the right policy instruments in the future. In addition, transparent certification methods must be developed to ensure the environmental benefits of CO₂-based chemical production in general, and especially for H₂-production and transport, because auxiliary processes can have a major impact on the overall performance. However, the integration of CO₂-based MeOH production into emission trading schemes will most probably not be sufficient to enable competitiveness. The calculated CO₂ avoidance costs are more than eight times higher than the actual (50 €/t CO₂ avoided, [80]) and expected carbon prices in the near future (85 €/t CO₂ avoided, [81]) within the European Union. Consequently, this policy instrument could possibly help to cover a minor part of the additional costs but is far from enabling competitiveness of CO₂-based MeOH production alone.

In general, current studies suggest that H₂ based on renewable electricity will most probably be a highly demanded resource in several industry sectors [6]. This enables synergies, i.e., to share the costs to set up a transportation and distribution infrastructure between multiple sectors, which reduces the import costs. Nevertheless, the build-up of international trading and transport infrastructure will be required to connect producing and consuming locations. Here, transport via ship constitutes a comparably expensive option for the short term because it requires less lead-times, whereas transport via pipelines is more promising in the mid- and long-term perspective. Nevertheless, both options should be pursued, because synergies and cost reductions due to technical development and learning curves could help the shipping pathways to reduce the transport costs. In addition, a more diversified import structure would help to reduce the independence from one supply source, and thus level supply risks.

The results of this study should be considered in the light of some limitations. First, the authors did not have access to the primary data of actual plants but had to derive the model parameters from literature data. In consequence, the modeling results can only approximate the described production processes, whereas in reality, different results may be reached. Nevertheless, the calculated uncertainty ranges help to understand in what range the real values would probably lie. Second, the concepts considered in this article are in part still hypothetical or only realized on a smaller scale. Scaling effects and synergies with other industries could lead to lower costs and a higher energy efficiency than the values considered in this study. Though scaling effects were estimated with the help of average scaling factors, market synergies were not part of the scope of this study. Furthermore, the effects of an increasing global demand for CO₂-based chemicals, which is expected to happen in the near future [82], were not considered in this study. This could enable regions and processes showing comparably high production costs to become competitive, too. Third, only one base chemical was considered as a case example. Other synthesis pathways, e.g., the use of H₂ and CO₂ to produce synthesis gas, offer the possibility to produce a broad range of CO₂-based base and high-value chemicals. They potentially provide a higher energy efficiency than MeOH-based synthesis and need H₂ directly. This could provide an advantage for the H₂ import pathways compared to the import of CO₂-based MeOH.

5. Conclusions

In this article, the combination of unavoidable CO₂ point sources in Germany with different import pathways for H₂ for CO₂-based MeOH production was assessed environmentally and economically. As case examples for H₂ provision, the hypothetical import via pipeline from Morocco and the currently under preparation import via ship from Australia were compared to possible domestic production using offshore wind as an energy source.

The results of the LCA show trade-offs between climate mitigation and other environmental impact categories for every pathway. They further show significant differences between the assessed alternatives, with the pathway for H₂ provision from electricity generation down to the delivery at the chemical plant being the most decisive factor. High transport and transformation efforts associated with the import of H₂ partly leveled more advantageous conditions for renewable energies in the exporting countries. Compared to the domestic production, environmental problem shifting by the import options studied in this article would result under the conditions of the status quo and in the near future.

From an economic perspective, production using electricity from an offshore wind park in Germany is more expensive than the import of H₂ via pipeline. Nevertheless, the domestic production would offer lower costs than most import pathways via ship in the status quo. For the import via ship, liquefied H₂ shows the highest costs. If the efforts for transformation processes and the short distance transport can be reduced in the future, all import pathways could exhibit lower or comparable costs than the analyzed production in Germany. With respect to climate change mitigation, import pathways via ship show the highest CO₂ avoidance costs. Thus, the climate mitigation effect is more cost-efficient for the production of CO₂-based MeOH using domestic H₂ production or the H₂ import via pipeline.

Compared with the import of CO₂-based hydrocarbons, the analyzed pathways show similar or higher environmental impacts and higher production costs now and in the near future. Thus, if CO₂-based MeOH cannot be produced in Germany, its import might be more favorable than the import of H₂ for chemical production.

To improve economic and environmental performance, the energy efficiencies of H₂-import pathways need to be increased in combination with a further decrease of investment costs along the whole value chain. Appropriate policies could complement this development and incentivize investments in this sector. For that, though, the hydrocarbon production pathways using imported H₂ must show that they can exhibit lower environmental impacts and costs than the import of CO₂-based hydrocarbons.

Future research should focus on technical development and process optimization as well as the analysis of suitable, effective, and economically efficient policy instruments. Furthermore, possible synergies with other industrial users of H₂ to reduce import costs could be analyzed.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/en15072507/s1>, Table S1: Process-specific energy and CO₂ demands and H₂ losses including the assumed values for the parameter range in form of triangle distributions; Table S2: General data and material balances for a 1 MW Proton Exchange Membrane Electrolyzer according to the status quo and the year 2030; Table S3: General data and material balances for the assumed H₂ liquefaction plant.; Table S4: Material balance for the hydrogenation and the dehydrogenation plants; Table S5: Material balance for a high-pressure storage tank used for H₂ tube trailers; Table S6: Composition of the assumed grid mixes for electricity in 2020 and 2030; Table S7: Description of Cost Parameters.; Table S8: Statistical parameters of the result distributions for the different footprints; respectively [83–100]. Figure S1: Box Plots showing the results distribution of the Monte Carlos for the Water and Land Footprints; Figure S2: Results of the sensitivity analysis for the production costs for the offshore, pipeline, and LH₂ pathway; Figure S3: Results of the sensitivity analysis for the production costs for both LOHC production pathways; Figure S4: CO₂-Avoidance costs for CO₂-based MeOH production in Germany for the year 2030, depending on the production costs and climate footprint of the used H₂.

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Nomenclature

AC	CO ₂ avoidance Costs
AUS	Australia
AWARE	Available Water Remaining
CCU	Carbon Dioxide Capture and Utilization
DE	Germany
FLH	Full Load Hours
FR	Fossil Reference
GHG	Green House Gases
GWI	Global Warming Impact
LCA	Life Cycle Assessment
LH ₂	Liquefied H ₂
LOHC	Liquid Organic Hydrogen Carriers
MCA	Monte Carlo Analysis
MeOH	Methanol
PV	Photovoltaic
PC	Production Costs
RMI	Raw Material Input
TMR	Total Material Requirement
wh	waste heat
WACC	Weighted Average Costs of Capital

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