Project no. 723678

‰The next Generation of Carbon for the Process Industry+

Coordination and Support Action

Theme [SPIRE 5] . Potential use of CO_2 and non-conventional fossil natural resources in Europe as feedstock for the process industry

Deliverable 4.3:

Economic and environmental impacts of most promising CCU pathways

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Organisation name of lead contractor for this deliverable: Trinomics (for the Economic part) and
Dechema (for the Environmental part)

1 Table of Contents

Objective of this Work Package and this Deliverable

This Work Package aims to assess the economic potential and environmental impact of selected CCU pathways. The selection of CCU pathways to be assessed (along with their technical feasibility) is presented in Deliverable 2.3. As part of this Work Package, two separate methodologies have been developed to support this assessment:

- Deliverable 4.1 providing the methodology to assess the business case and economic potential of a certain CCU pathway; and
- Deliverable 4.2 providing the methodology to assess the environmental impacts of the CCU pathways.

This Deliverable applies the methodologies to assess the selected pathways, and combines the results comparing the selected routes in terms of the economic and environmental results. The Deliverable consists of this report and an Excel tool, which provides the Greenhouse Gas (GHG) and cost assessments for all selected routes. The aim of this report is to present an overview of the results and to compare the different pathways from both an environmental and economic perspective. In addition, the report presents a brief analysis on key aspects regarding both the GHG and economic assessments. The results, in terms of the pathways showing the most favourable economic and environmental outcomes, are presented in Deliverable 4.4 rather than in this report.

Important note:

All the figures are rough estimates to give an indication of the attractiveness of a certain pathway. They can be compared but they do not aim to give any absolute values. We have used publicly available sources and data as much as possible. However, in reality, every project will have its own specific financial and environmental conditions. The excel tool (see 3.1) is designed in such a way that users can change the key variables in order to make more tailor-made estimates. For example, it is easy to add or change an economic or GHG scenario for energy and CO_2/CO supply. It is also possible to change input/output data of each of the processes used in the pathways. This will change the results automatically. This way, experts can refine the data collected in this project.

2 Methodology

This report contains the results from the economic and environmental modelling as described in the methodology deliverables D4.1 and D4.2 (Please refer to these deliverables for detailed information). This chapter will describe the overall approach and the connection and interaction between both methodologies and also the practical implementation.

2.1 General modelling approach

As mentioned in the preceding deliverables, CCU is a still a young field and many technologies do not exist on an industrial scale. Our main goal was to gather available data and create a framework and tool that could be used to compare different technologies at different TRLs and be able to update this tool when more information becomes available. It was also deemed important that the analysis is transparent and can be verified by external researchers. And finally, we wanted an integrated analysis for the economic and environmental analysis for consistency, but also easier updates.

All this led to the decision to create an Excel tool with the following parts:

- An overview of the selected pathways from work package 2 and all relevant data;
- A summary of all scenarios used;
- A collection of input-output data with literature sources for each process used in the pathways;
- An overview of each pathway, including the involved processes, emissions and costs for each scenario and reference technologies;
- Some utilities to treat and visualize this data.

The scenarios for the economic and environmental parts are independent of each other, as they have a different goal:

- The environmental scenarios are based on the IEA 2017 report for meeting the 2 °C target (International Energy Agency 2017) and the GaBi database[1] and show the greenhouse gas (GHG) intensity for the inputs hydrogen, electricity, heat and CO_2/CO in the years 2018, 2030, 2050 and for a "decarbonized world". Our study does not aim to show a scenario of GHG emissions evolution over time, but rather show the dependency of CCU pathways on low GHG

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[1] The GaBi database is a renowned commercial LCA database. In comparison to other databases, a lot of the data is based on real industrial process data.

energy. We therefore named the scenarios "EU Mix" (status quo), "RES~30 %"[2], "RES~80 %" and "Decarbonized".

- The economic scenarios on the other hand have as the main goal to compare the selected pathways with current market prices and among each other. Due to a lack of standardized methods, a variety of sources and methodologies is underpinning these estimations. Thus, the economic assessment presented here should be regarded as an estimate of how far the pathways are from attaining market competitiveness (price wise, when compared to current ways of production) and their relative economic attractiveness in relation to one another.

Textbox 1 Electricity mix and consequential LCA

This study is not an LCA, but most methodological choices are the same as for an LCA. One important choice, especially for processes consuming a lot of energy, is the energy supply. It is widely recognised that those CCU technologies are only low-carbon if low-carbon electricity is used.

Attributional vs. consequential LCA

An attributional LCAs are employed for current production routes in order to determine the environmental impacts for an already available product or service. Consequential LCAs are used to analyse the changes in environmental impacts that a change in production (volume, technology), consumption or disposing would incur.

As nearly all analysed CCU routes are not commercially available yet, the consequential LCA is the more obvious approach. Especially for large scale production capacities, CCU could significantly change the demand for electricity, hydrogen and heat.

Electricity mix in a consequential LCA model

In LCA terms, the electricity mix for consequential LCAs is often a *marginal* electricity mix (compared to an average mix in attributional LCAs), meaning the mix of electricity production facilities that have to be added to the current production mix to meet the demand of the new consumer. Even when considering to only use renewable electricity for CCU technologies, this renewable electricity could have been used somewhere else and could thus have avoided fossil power generation.

This is why this study presents selected results for the different energy scenarios to give an impression of the impacts associated with a pathway when this consequential view is adopted: that even when using renewable electricity, the marginal mix might still cause GHG emissions.

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[2] RES stands for "Renewable Energy System"

2.2 Selected pathways

The pathways selected for this study are based on deliverable 2.3 (available at http://carbonnext.eu/Deliverables.html), where they were selected based on the technology readiness level (TRL); market value; CO_2 or CO utilisation potential of the product and whether additional fossil carbon is used in the product. During the analysis, some modifications were made to the list, because either there was no data available for a specific pathway, or a more efficient pathway was found (e.g. the direct synthesis of Dimethyl ether was found to be more efficient than the "*condensation then dehydration of CO_2-derived methanol*").

Table 1 compares the pathways from deliverable 2.3 and the ones analysed in this deliverable.

The differences are essentially:

- The suppression of the second propylene pathway, because there was not enough data to accurately describe the two different pathways;
- A different pathway for dimethyl ether from CO_2, because it was found to be more efficient than the originally described pathway "DME production by condensation then dehydration of CO_2 derived methanol in the presence of a catalyst" (Keil 1999a);
- The addition of calcium carbonate as the only pathway that has a negligible energy input, as the formation of calcium carbonate is exothermic. It is an often described "low-hanging fruit" and can be seen as a carbon capture and storage or utilisation strategy depending on the use of the product;
- The suppression of the FT jet fuel pathway, as the differences to FT diesel and gasoline are small, but no data was found on those differences. As a first approximation, FT gasoline may be used.

The four pathways to produce methanol have been reduced to four pathways to produce syngas, and then the reforming routes have been split into one route using fossil methane and one using CO_2-based methane. Those six syngas routes have then been compared in chapter 3.1 for all pathways using syngas, not only the methanol pathways.

Table 1 Overview of selected pathways. Blue: chemicals, red: chemicals or fuels, yellow: fuels, white: solids

	Product	Pathway	Changes in this deliverable	Name in this deliverable
CO_2	Ethylene	Methanol to olefin (MTO) process (condensation of CO_2-derived methanol to DME followed by conversion to olefin)		Ethylene
	Propylene	Methanol to olefin (MTO) process (methanol plus ethylene)	No data found on the difference between the two MTO pathways	-
	Propylene	Methanol to olefin (MTO) process (condensation of CO_2-derived methanol to DME followed by conversion to olefin)		Propylene
	Ethylene carbonate	Carbonation of the epoxide ethylene oxide to ethylene carbonate		Ethylene carbonate
	Benzene	Methanol to aromatics (MTA) process developed by Mobil involving reacting methanol over a zeolite catalyst resulting in the simultaneous production of all three BTX components.		Benzene
	Xylene	Methanol to aromatics (MTA) process developed by Mobil involving reacting methanol over a zeolite catalyst resulting in the simultaneous production of all three BTX components.		Xylene
	Dimethyl ether	Condensation then dehydration of CO_2-derived methanol.	Used direct synthesis from syngas	Dimethyl ether
	Methanol	High temperature solid oxide cells use CO_2 and water to produce H_2 and CO, followed by compression and subsequent catalytic methanol synthesis.	Corrected the typo „FT synthesis" to „catalytic synthesis". Considered the four syngas production alternatives as described in chapter 3.1.	Methanol
		Dry reforming of CH_4 and CO_2 to produce syngas, followed by water gas shift reaction to adjust the CO:H_2 ratio, water removal, compression and subsequent methanol synthesis via catalytic synthesis.		
		Reverse water gas shift of CO_2 and renewable H_2 to produce CO and water, remove water, add more H_2, then use catalytic synthesis to produce methanol.		
		CO2/steam reforming of CH_4, followed by water gas shift reaction to adjust the CO:H_2 ratio, water removal, compression and subsequent methanol synthesis via catalytic synthesis.		
	Gasoline	Methanol to Gasoline process, via DME and olefins.		MTG Gasoline
	Gasoline	Syngas produced from CO_2 and H_2 undergoes F-T reaction at 300-350°C to produce gasoline-range hydrocarbons.		FT Gasoline
	Diesel	Syngas produced from CO_2 and H_2 undergoes F-T reaction at 200-240°C to produce linear waxes. Hydrocracking converts to synthetic diesel.		FT Diesel
	Methane	CO_2 methanation (Sabatier reaction)		Methane
	Calcium carbonate	Use carbon dioxide and steelmaking slags to produce precipitated calcium carbonate	Added the carbonation of calcium	Calcium carbonate

	Product	Pathway	Changes in this deliverable	Name in this deliverable
CO	Ethylene	Methanol to olefin (MTO) process (condensation of CO-derived methanol to DME followed by conversion to olefin)		Ethylene
	Propylene	Methanol to olefin (MTO) process (methanol plus ethylene)	No data found on the difference between the two MTO pathways	-
	Propylene	Methanol to olefin (MTO) process (condensation of CO-derived methanol to DME followed by conversion to olefin)		Propylene
	1,3-Butadiene	Gas fermentation of CO by the anaerobic bacterium Clostridium sp. Via 2,3-butanediol		1,3-Butadiene
	Benzene	Methanol to aromatics (MTA) process developed by Mobil involving reacting methanol over a zeolite catalyst resulting in the simultaneous production of all three BTX components.		Benzene
	Xylene	Methanol to aromatics (MTA) process developed by Mobil involving reacting methanol over a zeolite catalyst resulting in the simultaneous production of all three BTX components.		Xylene
	Dimethyl carbonate	Carbonylation of methanol in the presence of O_2		Dimethyl carbonate
	Ethanol	Gas fermentation of CO by the anaerobic bacterium Clostridium autoethanogenum.		Ethanol
	Methanol	CO and H_2 react over a Cu/ZnO catalyst		Methanol
	Dimethyl ether	Condensation then dehydration of CO-derived methanol in the presence of a solid acid catalyst		Dimethyl ether
	Gasoline	Methanol to Gasoline process, via DME and olefins.		MTG Gasoline
	Gasoline	CO and H_2 undergoes F-T reaction at 300-350°C to produce gasoline-range hydrocarbons.		FT Gasoline
	Diesel	CO and H_2 undergoes F-T reaction at 200-240°C to produce linear waxes. Hydrocracking converts to synthetic diesel.		FT Diesel
	Jetfuel - kerosene type (C_8H_{18} - $C_{16}H_{34}$, average $C_{12}H_{26}$)	F-T reaction to produce kerosene-type hydrocarbons	Not enough data found on FT for jetfuel	-
	Methane	CO methanation over a nickel catalyst.		Methane

2.3 Methodology for GHG assessment

There are some notable methodological choices when performing an environmental assessment of CCU technologies.

The first one is the choice of how to treat the CO_2 utilised in the process. Depending on the goal of the study, it could be credited to either the emitting process or the CCU process, or it could be allocated between both processes depending on a physical, technical or economic criterion. There could even be a distinction between fossil and biogenic CO_2. The goal of this study is to compare if it is better to use the CO_2 in a CCU process that would otherwise just be emitted, or if it is better to keep the conventional process, and compare different CCU pathways with each other. Therefore, we decided to credit the CO_2 utilised by the CCU process, but also burden it with emissions due to CO_2 capture and conditioning impacts. This means that in the balance sheet, all CO_2 being utilised in the product has a negative GHG emission (of -1 kg_CO_2-eq/kg_CO_2 utilised) because it is not emitted, but also a positive GHG emission determined by the energy consumption to capture that kg of CO_2. This choice is only valid as long as CO_2 is available from point sources and virtually "freely available", so that the CCU process only needs to care about the processes from capture onwards[3].

CO is treated in a similar way. It is assumed that CO is currently used to generate electricity on site, but if the CO is used in a CCU process, this electricity has to be produced elsewhere. However, in this instance the CO_2 emissions from burning the CO in a power plant are avoided. Burning 1 kg CO generates 1.57 kg CO_2, so we credit the avoided 1.57 kg CO_2/kg CO to the CO supply process, but burden it with the emissions of an equivalent electricity production of 1.53 kWh from the same scenario. Finally, we also add the emissions from CO capture and conditioning.

Table 2 summarizes the data used for each one of the scenarios analysed.

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[3] Capture, conditioning, transport and usage.

Table 2 Environmental scenarios

| GHG emissions		EU Mix	RES~30 %	RES~80 %	Decarbonized
Electricity [kg CO₂eq/kWh]		0.44	0.15	0.06	0.01
H₂ [kg CO₂eq/kg H₂]		10.70	7.58	2.14	0.67[4]
heat [kg CO₂eq/kWh]		0.26	0.16	0.04	0.01
CO₂ [kg CO₂eq/kg CO₂]	**Credit**			-1.00	
	Capture	0.15	0.23[5]	0.06	0.02
	CO₂ balance	-0.85	-0.77	-0.94	-0.98
CO [kg CO₂eq/kg CO]	**Credit**			-1.57	
Capture and electricity replacement		0.82	0.28	0.11	0.02
CO balance		-0.75	-1.29	-1.46	-1.55

2.4 Methodology for estimating economic performance per pathway

The figure below represents the schematic representation of the overall approach for estimating the economic performance per pathway. Each component of the approach is explained in detail below.

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[4] For hydrogen production, the source of the scenarios (Jan Koj *et al.* 2017) considers an electricity consumption of 50 kWh/kg hydrogen. Additionally, the electrolyser production has noticeable GHG emissions.

[5] The emissions for the capture process increase compared to the current EU mix because the literature source assumed a switch from coal fired power plants to direct air capture (due to a higher demand of CO_2 than available point source supply).
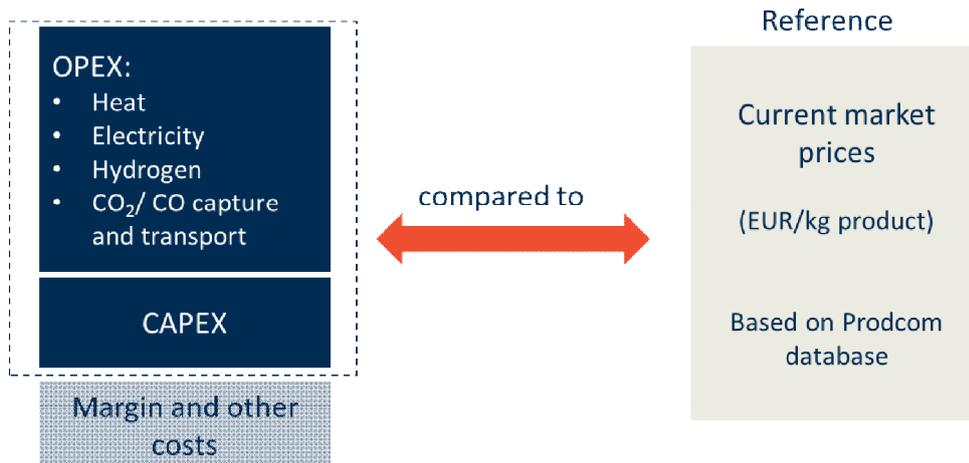
Figure 1 Schematic representation of the overall approach to estimating the economic performance per pathway. The production costs (OPEX and CAPEX) of each pathway are compared to the current market price of the product (produced by a conventional method)

Capital expenditure

Capital expenditure (CAPEX) refers to costs associated with non-consumable parts of the process (e.g. equipment, machinery etc.). Estimating the CAPEX of the CCU pathways selected in deliverable 2.3 is challenging because many of these pathways have not yet reached commercial maturity and there is limited information available in literature. Therefore, all CAPEX figures should be treated as rough estimations only. In order to be consistent across the GHG and the economic estimates, the scope of the CAPEX was selected in a way consistent with the GHG assessment.

The CAPEX for the final pathways selected in deliverable 2.3 and summarized in annex A were calculated based on the material flow analysis in the Excel tool. Thus, the final CAPEX per pathway was calculated by adding the CAPEX for each specific step multiplied by the multiplicator[6] for that step in each pathway. A CAPEX for the different ways of producing syngas was included in the analysis for syngas dependent processes. The scope for the CAPEX excluded sources of hydrogen, carbon monoxide and carbon dioxide. These costs are already included in the prices for the materials under operational expenditures (OPEX).

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[6] The multiplicator is used to build the pathways from process steps. If the input of the final process step is produced by another process, the multiplicator defines the ratio of needed input to produced output of the two processes. IF for example a MTA process would need 4.3 kg of methanol to produce 1 kg of aromatics, and the methanol producing process was defined for 1 kg of methanol, the multiplicator would be 4.3 (see also deliverable 4.2, chapter 4.1.2).

Operational expenditure

The operational expenditure (OPEX) is calculated based on the following main cost components:

- Electricity cost;
- Heat cost;
- Hydrogen cost;
- CO_2 or CO capture and transport cost.

These are calculated using the following assumptions used in each of the scenarios described in the methodology (See Deliverable 4.1 for more details). Further, prices for heat are based on gas wholesale prices adjusted with a conversion factor of 90% and an additional 35% operation costs. CO_2 and CO capture and transport costs are based on the costs identified in Deliverable 3.1. For CO, expert opinion and an additional proxy assessment based on gas wholesale prices was used (comparing the energy content per mole for natural gas and CO, and adjusting the price accordingly).

Table 3 Economic scenarios for 2030

2030 prices	Scenario 1 Most unfavourable	Scenario 2 High H_2, low E and heat	Scenario 3 Low H_2, high E and heat	Scenario 4 Most favourable
H_2 price [Ö/kg H_2]	6	6	2	2
Electricity price [Ö/kWh]	0.140	0.059	0.140	0.059
Heat price [Ö/kWh]	0.057	0.03	0.057	0.03
CO_2 capture and transport cost [Ö/kg CO_2-eq]	0.045	0.022	0.045	0.022
CO capture and transport cost (Ö/kg)	0.01	0.01	0.006	0.006

Comparison with current market prices

The production cost (estimated as OPEX + CAPEX per unit produced) of the pathway will be compared to the price of the fossil-based alternative that is already on the market. This allows for comparison across pathways and between the conventional way of production versus the CCU pathway.

For most products, the current market price is calculated based on the market value and volumes which are available in the PRODCOM database. For those products which have no data available in

the PRODCOM database we have used indicative market prices from other sources. These values and the sources are listed in annex C.

Comparing this market price to the production cost of the CCU pathway gives an indication of the competitiveness of the CCU product if it would enter the market. It only gives an indication, as we do not know the future market price of the CCU product: the production cost needs to be complemented with overhead costs, other consumables, margins, etc. to arrive at the true market price. Because of these other elements, the market price can be substantially higher than the production cost: some of the products, for example, can have margins of 25%.

2.5 Assumptions and data gaps

Data availability for the low TRL processes is always a hurdle in Techno-Economic Analysis (TEA) and LCA. We were able to find either TEA or LCA studies for most of the processes, but most of the time, the publications did not openly disclose the sources or all inputs and outputs or costs of the process. A lot of the processes are commercially confidential, patented or in the process of being patented.

We believe that the following processes contain the biggest gaps or highest uncertainty for the inventories:

- The LCA for Fischer Tropsch process is quite well studied, but most studies use biomass as input. Also, the difference between diesel, gasoline and kerosene as output are hard to find.
- The CO gas fermentation process is a proprietary process and the available information does not always allow getting the inventory in the way needed for the Excel tool. Also, there is little to no information on the 1,3-Butadiene process alternative.

For CAPEX, the highest uncertainties stem from the fact that the selected pathways have not yet reached commercial maturity. The CAPEX estimates for the processes used to construct full pathways are listed in annex A. These values were either taken directly from literature or derived from information in literature based on capital investment costs and production rates for existing or modelled (theoretical) industrial plants. In those cases where the plant lifespan was not explicitly stated in literature, a 12-year lifespan was assumed.

Based on the descriptions of the industrial processes for these routes, it was assumed that the CAPEX of the methanol-to-aromatics (MTA), methanol-to-olefins (MTO) and methanol-to-gasoline (MTG) processes will be very similar. Due to lack of available information, the CAPEX for the MTA process was estimated from literature and applied for the MTO and MTG processes equally.

3 Overview of results

This section provides an overview of the results from the GHG and economic assessments, which are provided in detail in the Excel tool accompanying this report. In order to facilitate comparison, this chapter makes use of one cumulative value for the GHG results and one for economic impact. These metrics are:

- **Absolute GHG emissions compared to reference**. The GHG emissions are determined by adding the process CO_2 balance plus the GHG emissions for electricity, heat, hydrogen, CO_2 and CO production and/or supply.
- **Overall costs in Euros per kilogram of final product**. The costs for each pathway are determined as the aggregated CAPEX and OPEX (including H_2, CO, CO_2, electricity and heat costs).

3.1 Syngas and methanol as building blocks

Most of the pathways use platform chemicals as building blocks. The most common platform chemicals in this study are syngas (predominantly H_2 and CO), methanol and methane. These are already widely used in the current chemical industry.

Syngas can be produced via multiple routes. We analysed the following processes to produce syngas:

- **High temperature solid oxide cells** (HT SOC): $2\,CO_2 + 2\,H_2O \rightleftharpoons 2\,CO + 2\,H_2\,(+\,O_2)$
- **Dry reforming of methane**: $CH_4 + CO_2 \rightleftharpoons 2\,CO + 2\,H_2$
- **Reverse water gas shift** (rWGS) of CO_2 and renewable H_2 to produce CO and water, remove water, add more hydrogen: $CO_2 + H_2 \rightleftharpoons CO + H_2O$, $CO + H_2$
- **CO_2/steam reforming of methane**: At high temperatures (850-1000 °C) steam and CO_2 react with methane to produce syngas via the following reactions:
  $CH_4 + H_2O \rightleftharpoons CO + 3\,H_2$
  $CH_4 + CO_2 \rightleftharpoons 2\,CO + 2\,H_2$
- **Mix CO as input with renewable H_2**

The last process is only relevant for CO based pathways (e.g. from steel mills).

For the two reforming routes of methane, methane can either come from CO_2 via the Sabatier process or from fossil sources. This gives a total of 6 routes to produce syngas from CO_2, and only one route from CO.

It is important to note that the ratio of produced hydrogen to CO is different depending on the syngas production route of choice. CO_2/steam reforming of methane has the highest ration of H_2 production in

relation to CO, followed by HT SOC and dry reforming. In contrast, reverse WGS does not produce hydrogen, so hydrogen has to be added.

Methanol (MeOH) can then be produced from syngas from all of the above processes. There are some technology developments to directly produce methanol from CO_2 and H_2, but they were not selected for assessment at this time because of their low TRL. Figure 2 shows all the pathways that start with syngas.
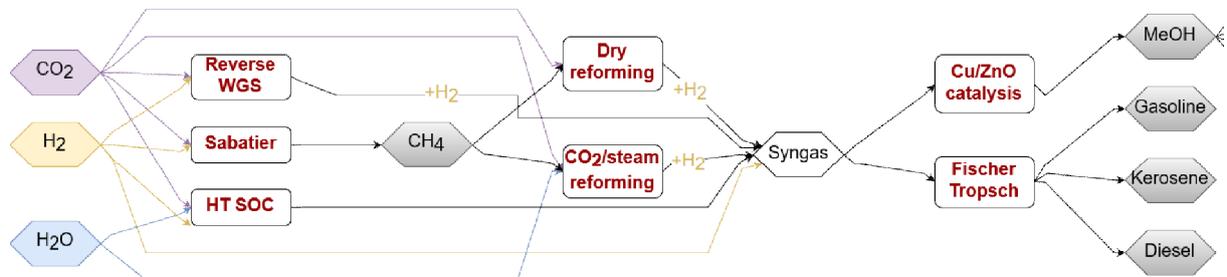
Figure 2: pathways starting with syngas

Figure 3 shows the pathways that use methanol as an intermediate product (produced from one of the syngas processes above as shown on the top right in Figure 2). Altogether, 10 out of 12 analysed pathways from CO_2 are using syngas as a building block.
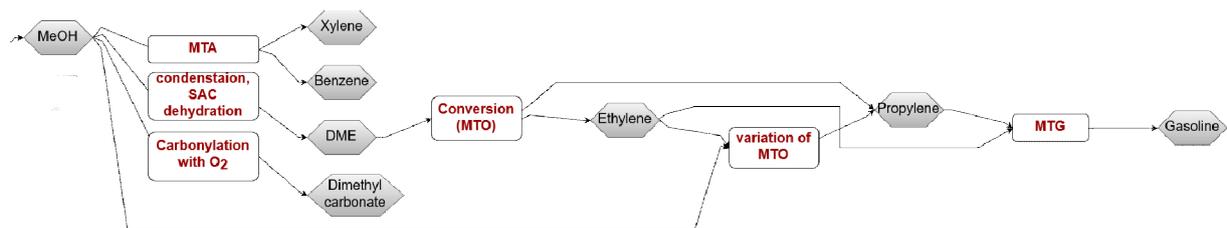
Figure 3: pathways from methanol

Because of the importance of syngas, we analysed the impact of the syngas production on the different processes both within the GHG and business assessment.

3.1.1 Environmental impact of syngas routes

The environmental impact of syngas routes strongly depends on the electricity and hydrogen production. Figure 4 shows the GHG emissions for all six routes and for the four energy scenarios:

- **EU Mix**: current European electricity, heat and hydrogen production
- **RES~30 %:** electricity GHG intensity drops from 0.44 kg CO_2/kWh to 0.15 kg CO_2/kWh, hydrogen and heat are mostly produced from electricity
- **RES~80 %:** electricity GHG intensity of 0.06 kg CO_2/kWh
- **Decarbonized**: wind power-based electricity with 0.01 kg CO_2/kWh
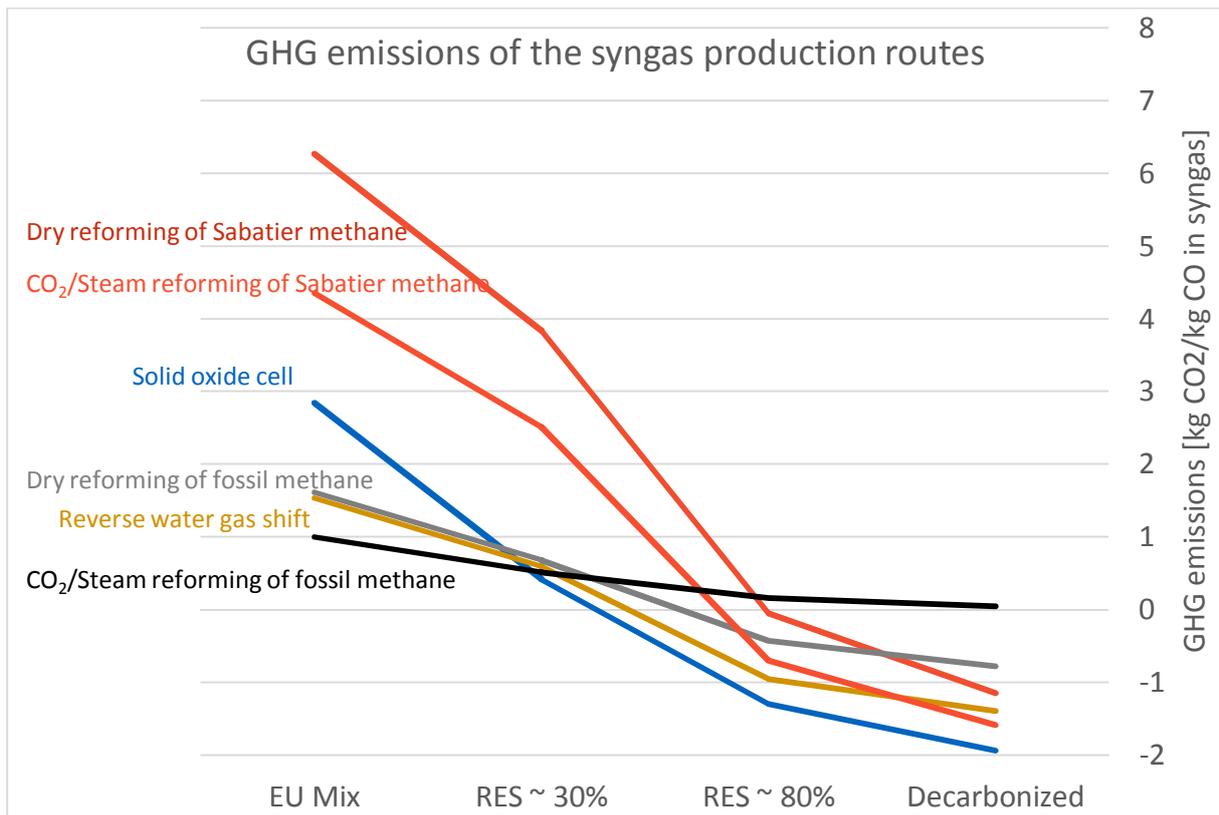
Figure 4: GHG emissions of the six syngas production routes from CO_2

When using decarbonized energy for CCU processes, the GHG impact of all syngas routes is quite close except for the two fossil methane reforming routes (which have higher emissions). On the other hand, as long as the used electricity mix has a GHG intensity of over 0.2 kg CO_2/kWh, the fossil methane reforming routes emit less GHG than the other routes (except reverse Water Gas Shift (rWGS)). The steepness of the curve when comparing the routes using the current energy mix towards a less GHG intensive electricity production can also be seen as a measure of the amount of electricity needed for each process because processes with a higher electricity demand show greater decreases in GHG emissions as the electricity supply is decarbonised.

Please note that the data presented here is based on TEA and LCA studies from the literature at different TRL levels. Even if a stoichiometric conversion from CO_2 to CO would lead to a maximum CO_2 uptake of 1.57 kg CO_2/kg CO in syngas, especially the solid oxide cell seems to have a higher uptake. This may be a measurement error, or it might mean that carbon is stored in the system.

3.1.2 Economic impact of syngas routes

This section provides an overview of the impacts of the four syngas routes on the business case of selected pathways. When comparing the production of syngas, CO_2 steam reforming of Sabatier methane is the most expensive route for all but one scenario. The price differences between production via the reverse water gas shift route and dry reforming are minimal, though reverse water

gas shift performs slightly better in all the economic scenarios assessed. In comparison to these three routes, which are sensitive to hydrogen prices, the production of syngas via high temperature solid oxide cells (HT SOC) is very sensitive to electricity prices.
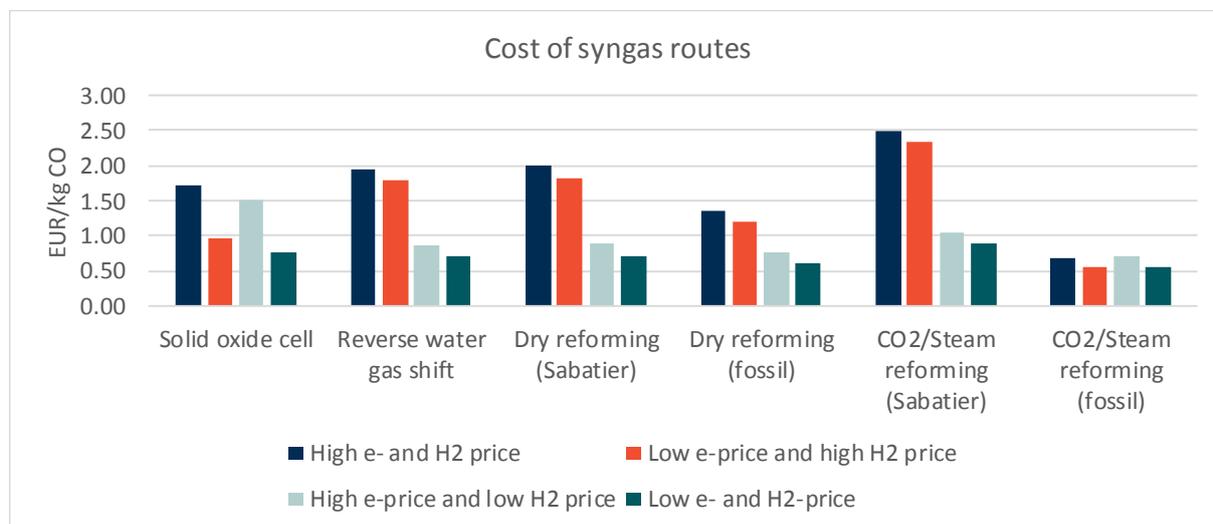
Figure 5 Costs of syngas (EUR/ 1kg CO and 0.2 kg H_2) per route and economic scenario

The economic analysis shows that for syngas-dependent pathways (see Figure 2), the choice of syngas production route has a significant impact on the total costs. Based on the material flow analysis, (see the Excel tool) it is apparent that production of syngas using HT SOC is the most electricity and heat intensive process and also requires the largest CO_2 input out of all processes. However, this is the only syngas production pathway which does not require H_2 input. Thus, high electricity and heat prices have significant effects on the total cost of this pathway. On the other hand, high H_2 prices will not affect the total cost of syngas production via solid oxide electrolysis. Syngas production via dry reforming of methane does not require heat input, but is sensitive to electricity, CO_2 and H_2 prices. On the other hand, reverse water gas shift and steam reforming of methane to produce syngas are both sensitive to changes in all assessed prices (i.e. heat, electricity, CO_2 and H_2). Depending on the scenario, the HT SOC and reverse water gas shift routes are the cheapest.

3.1.3 Summary of syngas routes

Producing syngas is an important process in most analysed CCU processes from CO_2. The best economic and environmental syngas route depends a lot on the scenario assumptions, i.e. the electricity and hydrogen price and environmental impact. CO_2/steam reforming of Sabatier methane and high temperature solid oxide cells (HT SOC) have the lowest environmental impact if decarbonized energy is used, but especially HT SOC has the highest impact for the current energy mix, while reverse water gas shift (rWGS) is quite good for every energy mix. As the costs are also largely determined by the energy input, the best economic routes are also HT SOC and rWGS

depending on the economic scenarios (though the cost differences between rWGS and dry reforming of Sabatier methane are minimal).

An important point to keep in mind is that the H_2/CO ratio is not the same for all routes. Especially rWGS has no hydrogen in the output and needs to add additional hydrogen up to the ratio needed by a given process. On the other hand, HT SOC has about 13 wt-%[7] and CO_2/steam reforming around 18 wt-% of hydrogen. If the following process needs less hydrogen, this has to be adjusted after the syngas production. In this study, we assumed that the H_2/CO ratio would be adjusted by:

- either a rWGS process between the syngas producing route and the following process to reduce the hydrogen content,
- or by adding hydrogen from the scenarios to the syngas.

When looking at a pathway in detail, it is important to use the best syngas route and to check how best to adapt the H_2/CO ratio. Since the main motivation behind CCU is to reduce GHG emissions and broaden the raw material base and since the current costs for all syngas pathways analysed are significantly higher than the conventional ways of production, the rest of the economic analysis focuses on HT SOC and rWGS because they tend to have the lowest costs while having the lowest GHG emissions. Nevertheless, depending on the energy scenario, another syngas route might be a better choice.

## 3.2 Results for all pathways

The following sections provide a comprehensive overview of the results for both the environmental and economic assessments.

3.2.1 Environmental assessment overview

Figure 6 shows the range of GHG emissions for all pathways over all scenarios and syngas routes, compared to the range of GHG emissions of the reference over all scenarios. A large range indicates that the pathway uses a lot of energy inputs (hydrogen, electricity, heat) and thus depends on decarbonized energy to be able to compete with the GHG emissions of the reference. Some pathways (like ethylene carbonate and calcium carbonate from CO_2 or ethanol and methanol from CO) have a narrow range because the chemical reaction does not require a lot of energy. Others like ethylene, propylene, xylene or benzene have a high energy consumption, but can save GHG emissions if this energy is decarbonized.

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[7] Weight-%. For HT SOC, 1 kg of syngas contains 0.87 kg of CO and 0.13 kg of H_2.
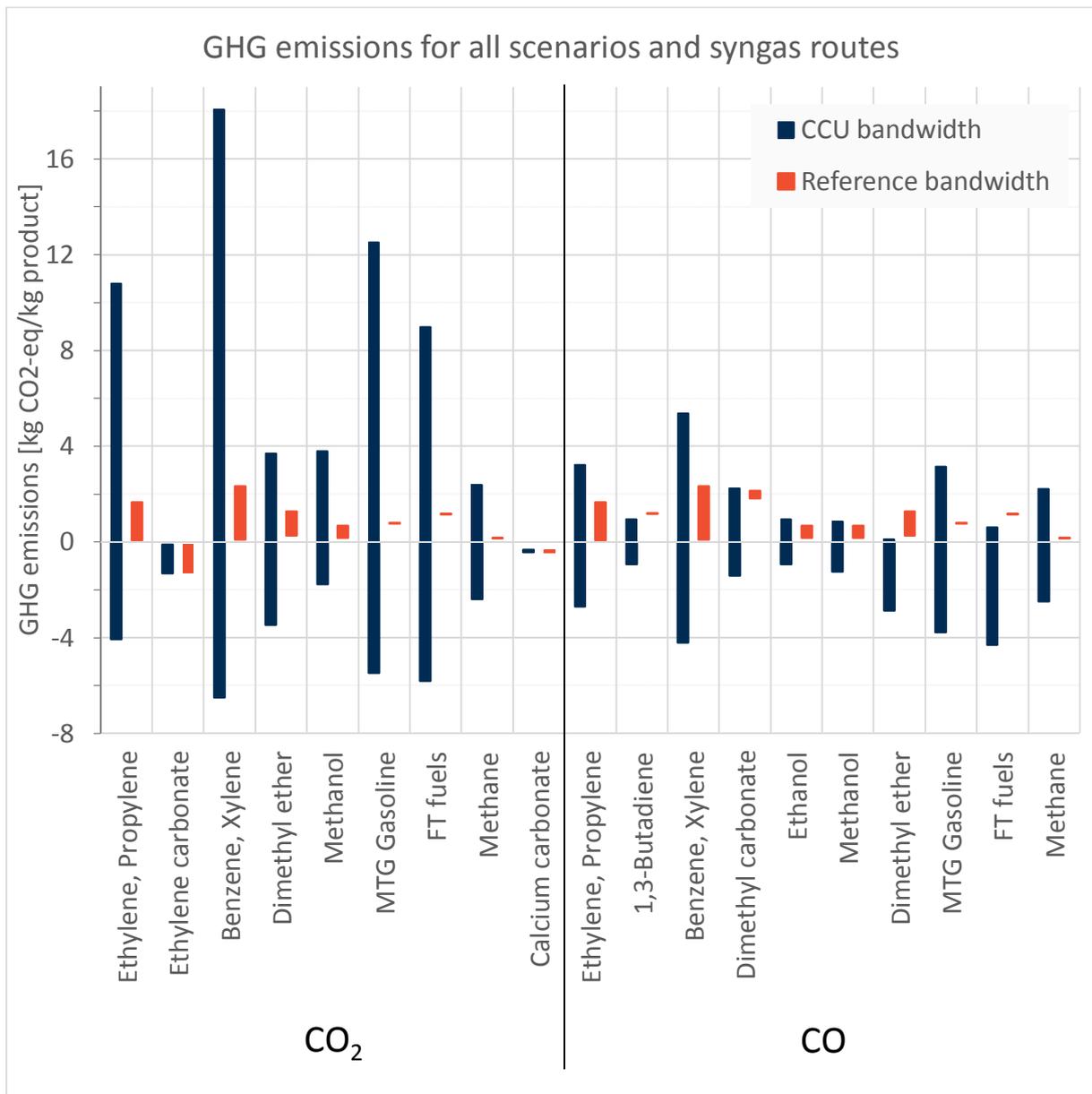
Figure 6: Overview over GHG emissions for all pathways compared to the reference Ë range over all scenarios and syngas routes. For details, see Figure 9.

All pathways benefit from the GHG credit of the CO or CO_2 incorporated into the product and have lower GHG emissions than their reference in the Decarbonized energy scenario. Different pathways have different proportions of inputs (CO, CO_2, hydrogen and energy supply: heat/electricity), which influences the break-even point with the reference technology.

For pathways from CO_2 for example, if using syngas from CO_2/steam reforming of fossil methane, DME, FT fuels and methanol might already have lower GHG emissions with today's energy mix than

the reference[8]. Other pathways, especially for more complex molecules like olefins or aromatics, use more electricity, heat and hydrogen and only emit less GHG than the reference with approximately 80-90 % of renewables in the energy mix. But once the energy mix is decarbonized, they can save more GHG than the shorter molecules. Energy input for those pathways is high, so it is important to keep in mind renewable energy availability when looking at large-scale deployment.

For CO based pathways, all pathways can save GHG emissions with as little as 50 % of renewables in the energy mix[9]. Again, longer molecules can incorporate more carbon per kg of product and therefore have a higher GHG reduction potential if produced with decarbonized energy. As CO has a higher energy content than CO_2, most pathways use less electricity and heat than the CO_2 pathways and are less dependent on a high renewable energy share.

3.2.2 Economic assessment overview

The economic assessment shows the range of costs, accounting for all scenarios and syngas routes. It shows that for most products, the CCU pathways have a much higher cost (up to almost 1500% more) than the current market price, and that only for very few pathways the costs can be close or even lower than the market price. In the next chapter (5) we analyse the main drivers causing these important price differences.

The following diagram shows the range of costs for the different pathways and their current market price. The bars represent the range between the lowest and highest production cost for 1kg of product from the different combinations of scenarios and syngas routes per pathway, taking into account CAPEX and OPEX.

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[8] But as one goal of CCU is to reduce the dependency of the chemical industry on fossil sources, reforming of fossil methane is not seen as the right solution.

[9] %Energy mix+means electricity, heat and hydrogen as well as CO capture and conditioning.
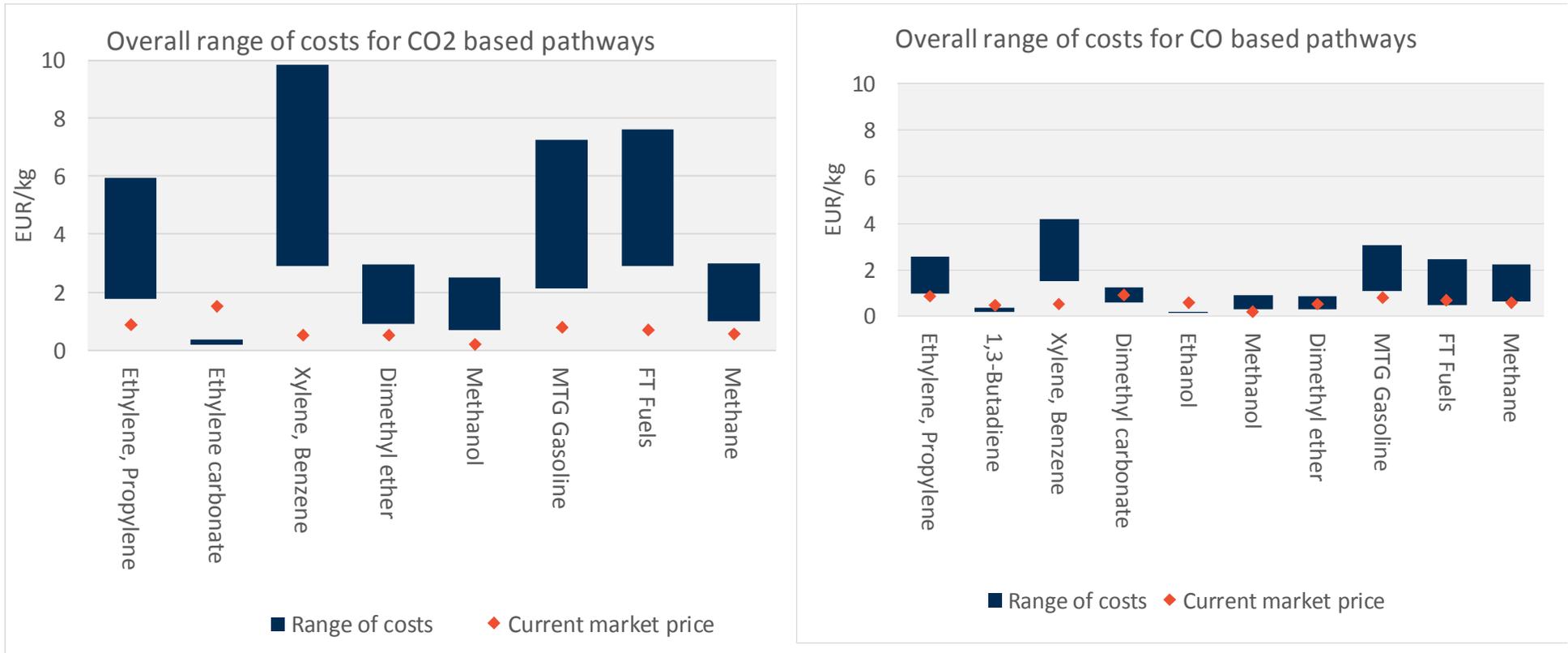
Figure 7 Range of costs for the different pathways for all economic scenarios and syngas routes

From this diagram it can be noted that:

- **In a few cases we find competitive results across all pathways and syngas routes** (ethylene carbonate, 1,3-butadiene and ethanol), where the assessed costs are always under the current market price. However, this does not mean that we expect these routes to be necessarily more profitable than the conventional pathways by 2030. As mentioned earlier on, our assessed costs are only indicative and do not account for a profit margin and several other costs. Moreover, in the case of other products, certain combinations of scenarios and syngas routes result in costs that are lower than or comparable to the current market price (ethylene, dimethyl carbonate, dimethyl ether made using CO, MTG gasoline, FT fuels and methane made using CO).

- **The CO-based pathways seem to have lower costs overall** than CO_2-based pathways. The overall higher energy needs for CO_2-based pathways cannot compete with the CO pathways. Further, we see that for several CO-based pathways there is at least one economic scenario where the costs assessed are under the current market prices (e.g. dimethyl carbonate, dimethyl ether, gasoline and diesel).

- **FT fuel and MTG gasoline pathways have very high costs** in comparison to the rest of the pathways. This can be explained by the cost of hydrogen and the strong need for additional energy (electricity).

4 Environmental impacts . GHG emissions

4.1 Main GHG drivers

As described before, most CCU pathways are greatly impacted by electricity and hydrogen production. Therefore, a big part of the GHG impacts come from the processes supplying those feedstocks. This can be seen in Figure 8[10] showing the breakdown for different pathways. The only two notable exceptions are the carbonation (of methanol and calcium) and fermentation processes as the one shown in Figure 8 d) for 1,3-butadiene. Fermentation processes (like 1,3-butadiene in d)) have very low energy inputs, but cause direct CO_2 emissions produced by the fermentation.

Parts a) and b) show the influence of the syngas route on most pathways, illustrated for methanol. While "CO_2/steam reforming of fossil CH_4" allows for lower GHG emissions with the current energy mix, it can only save about 0.3 kg CO_2-eq with the Decarbonized energy mix. rWGS on the other hand causes about 3 kg CO_2-eq more with the current energy mix, but can save up to 1.5 kg CO_2-eq with decarbonized energy.

For FT diesel in c), hydrogen supply is the only cause for GHG emissions. The process can produce electricity, which has been treated as a GHG credit (1 kWh of produced electricity was assumed to save as much GHG as 1 kWh of consumed electricity would cause in the scenario).

The reason that CCU processes can have lower GHG emissions than the reference is the CO_2 credit for the uptake of CO or CO_2 as explained in the methodology deliverable D4.2.

As explained in Textbox 1, it is important to consider the regional electricity mix for a new electricity consuming technology like CCU, even if the process is only using renewable electricity. This is why different energy scenarios are presented all along this report. In Figure 8, it is shown that the assumptions in those energy scenarios have a tremendous impact on the GHG emissions of CCU technologies. They also have an impact on the conventional reference processes that use electricity and heat (and some also hydrogen). For user convenience, we added a fifth energy scenario "Custom" to the Excel tool, which can be adapted by the user. In Figure 8, the Custom scenario has zero GHG emissions for all inputs and can be seen as a theoretical minimum for a pathway.

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[10] Figure 8 presents a selection of four pathways to highlight some interesting points. For detailed results per pathway, please refer to the Excel tool.
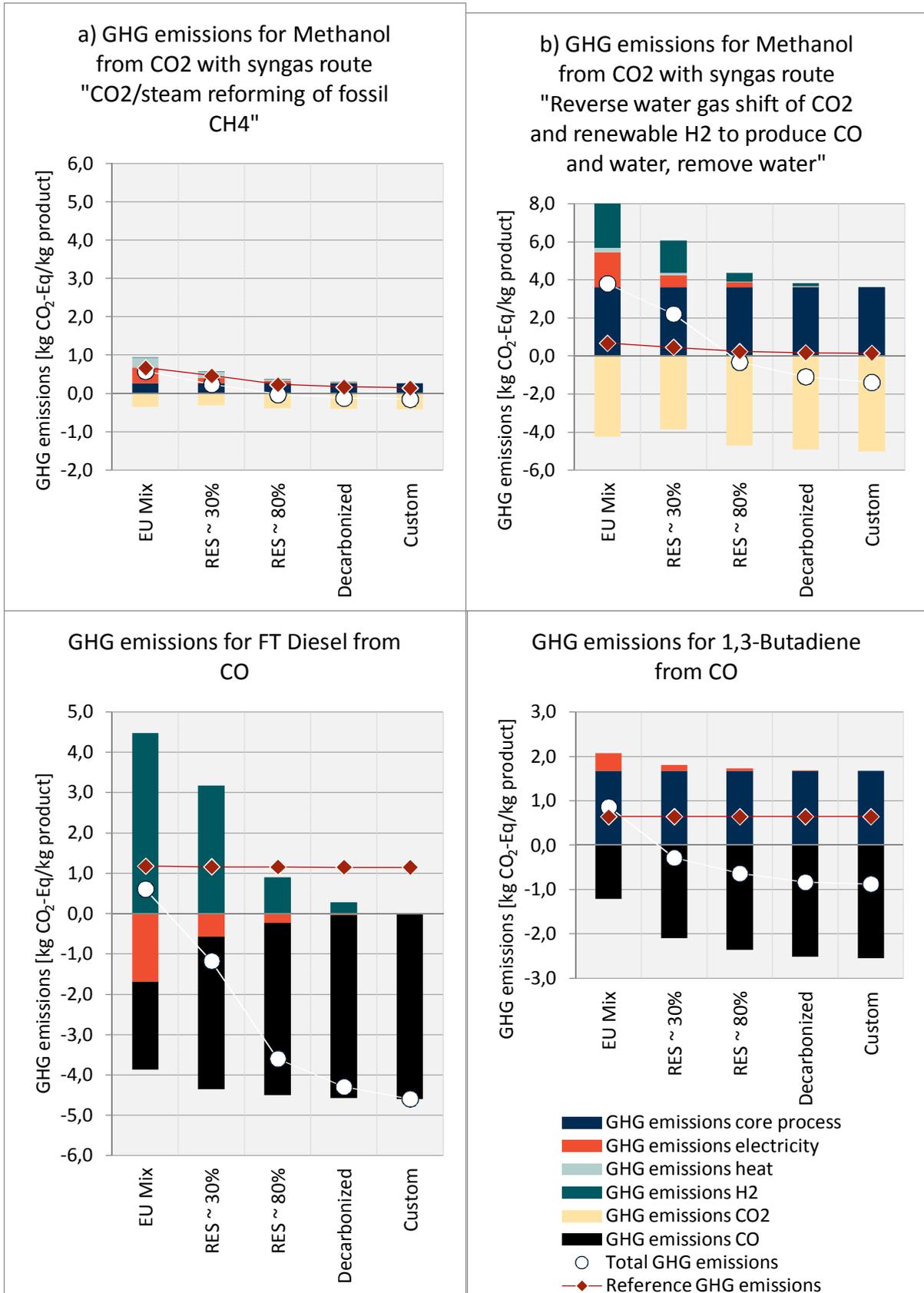
**Figure 8: Breakdown of GHG emissions for different pathways**

Figure 9 shows the increase or decrease of GHG emissions when replacing a conventional route with a CCU route to produce all selected products for all scenarios and all syngas production pathways. The colour indicates the energy scenario, while the shade determines the syngas route. As CO based pathways don't have different syngas routes, there is only one value per scenario.

The range of GHG difference within one scenario can be quite high, as for example for FT fuels from CO_2 in the "EU Mix+" scenario, where the worst syngas route causes roughly 8 kg more CO_2-eq than the reference, while the best route can save 1 kg of CO_2-eq.

Most pathways using CO_2 as carbon source are better than their reference with a reasonably clean energy mix corresponding to 50-80 % renewable electricity and hydrogen. The pathways that are better than their reference with lower percentage of renewable energies are DME, FT fuels and methanol. The high maximum GHG savings of aromatics (xylene and benzene) and olefins (ethylene and propylene) are caused by their capacity to incorporate nearly three times as much CO_2 per kg of product than for example methanol.

For CCU from CO, there is only one route for the production of syngas: adding hydrogen from electrolysis to the CO. The main cause of GHG emissions of those CCU pathways is the hydrogen production. Some pathways which do not need hydrogen are already better than the reference with the current EU electricity mix: DME, FT fuels and ethanol as well as 1,3-butadiene from fermentation. The highest possible GHG savings compared to the reference with decarbonized energy are again possible with FT and MTG fuels, aromatics, olefins and dimethyl carbonate.

This analysis provides a methodology to enable the comparison of the likely GHG emissions associated with different CCU technologies and pathways. We would like to remind the reader that this analysis is based on a heterogenous mix of TEA and LCA studies supplemented by our own conversions, calculations and assumptions. The results are meant to show a methodology to compare different technologies and to give very rough trends. For example, longer molecules can generally incorporate more carbon per kg of product and thus have a higher GHG reduction potential with decarbonized energy. Higher hydrogen content in the product (like for methane) generally causes higher GHG emissions.
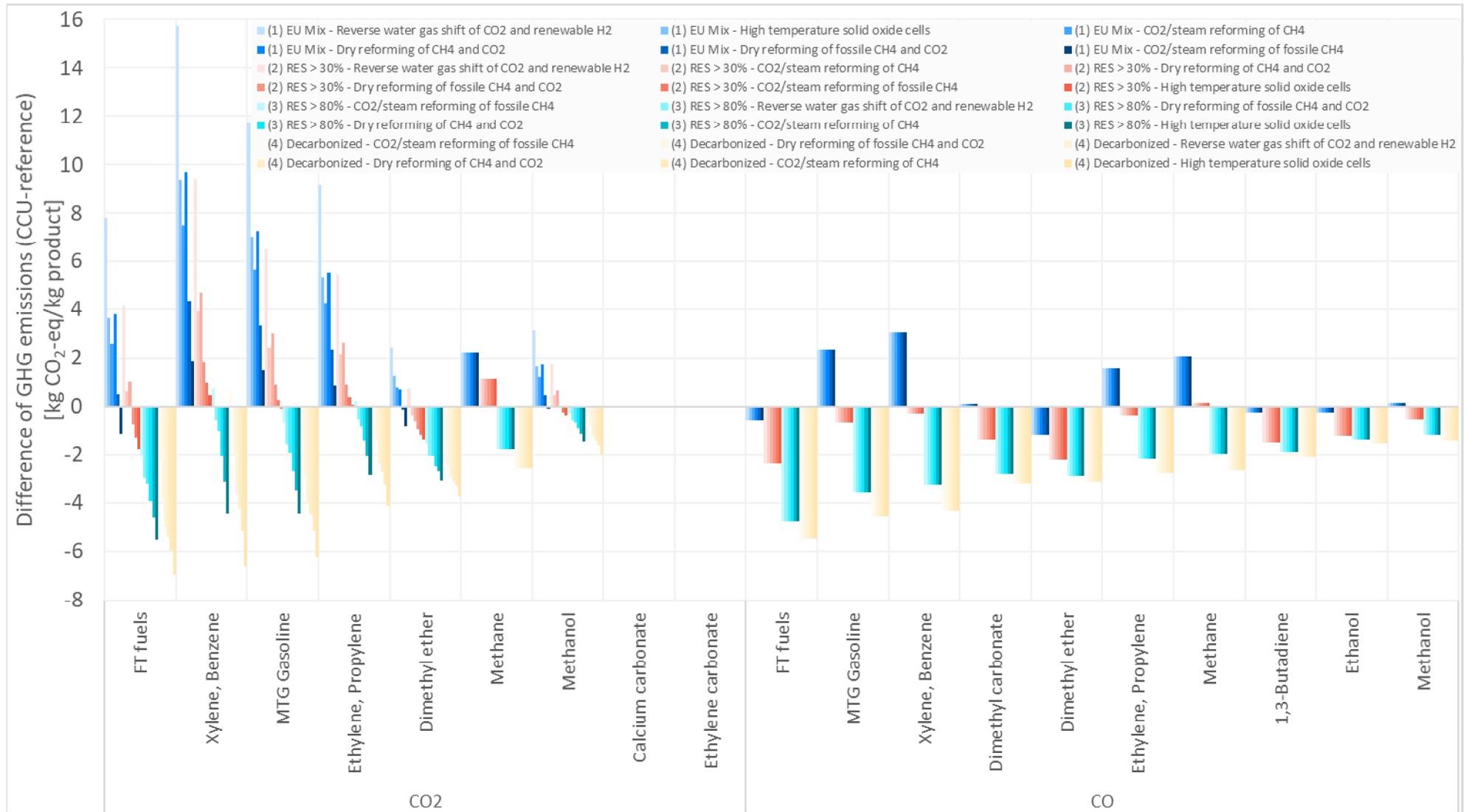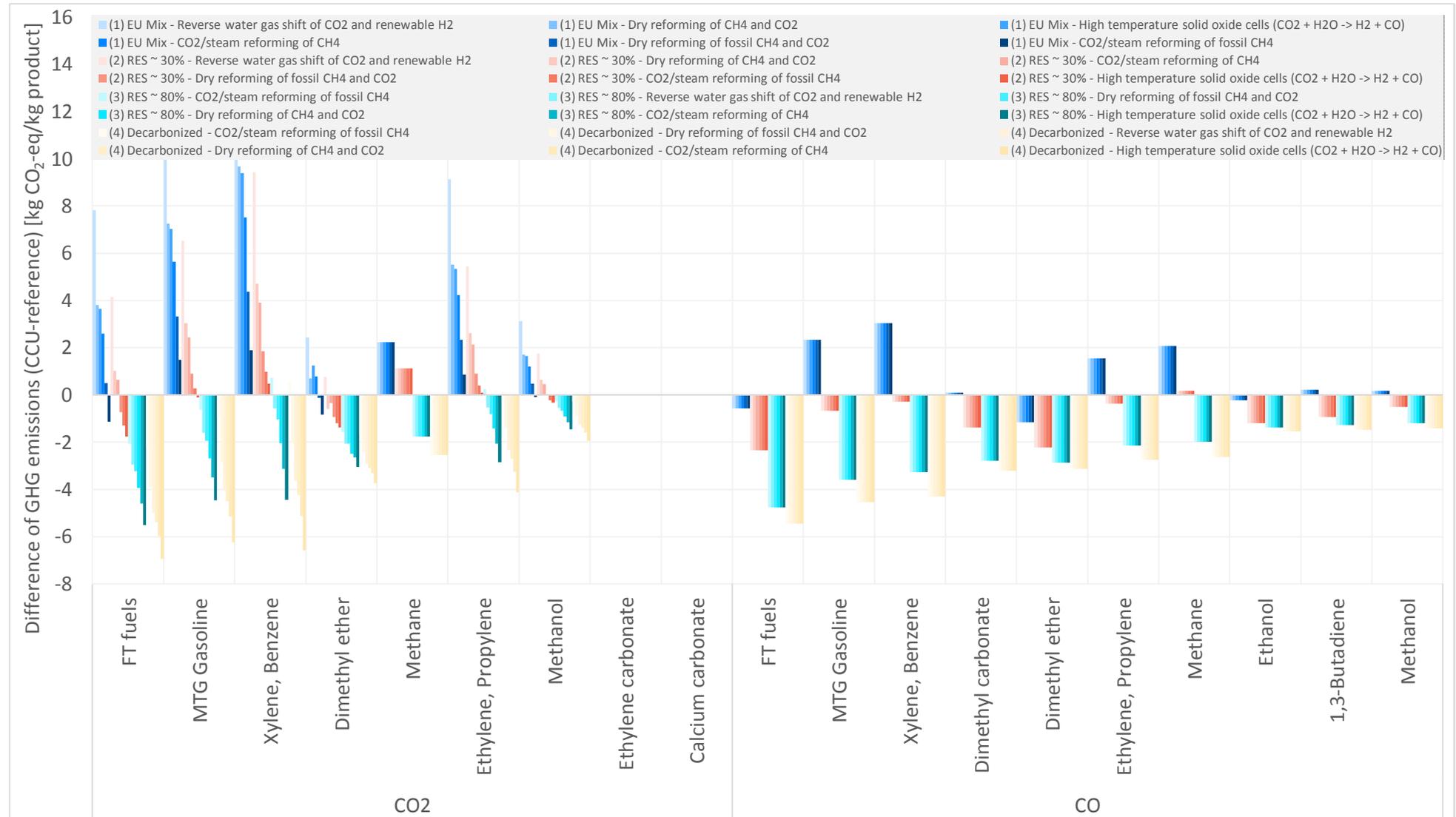
Figure 9: Change in GHG emissions compared to conventional route. Scenarios: blue for EU Mix, red for RES~30 %, turquoise for RES~80 % and yellow for decarbonized. Products sorted by highest total GHG savings in the Decarbonized scenario.

Textbox 2: Comparison with other studies

One similar study is that of (Bazzanella and Ausfelder 2017), who compiled a lot of data on CCU processes, including costs and CO_2 emissions. Compared to that study, the values presented here are generally in a similar range. One difference is the CO_2 capture and separation which is assumed to have higher GHG emissions in their study than in this study. They write that their assumption of 0.42 kg CO_2 per kg of CO_2 captured is "relatively conservative" and assume that the electricity needed for the capture is produced by the coal power plant that is also used as CO_2 source. This study, on the other hand, assumed that the electricity comes from the energy scenarios.

4.2 Selection of best environmental pathways

The choice of the best pathway depends largely on the metrics used. The set of best pathways when focusing on GHG reduction per kg of product yields is different than the one obtained when focusing on GHG reduction per kWh of electricity used or per kg hydrogen used. Figure 10 shows the different pathways organised by GHG reduction per kg of product (with the best pathways on the left side of each category: CO, CO_2). However, for CO_2 based pathways, high GHG reductions come with high electricity (or hydrogen[11]) consumption. CO based pathways on the other hand have generally a high hydrogen consumption. As those resources will always be limited and expensive, trade-offs will have to be made[12].

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[11] Not shown in Figure 10, because the syngas route with the lowest hydrogen consumption is shown.

[12] FT fuels from CO_2 seem to be the exception, but the only syngas route where surplus electricity is generated is from fossil methane, which is not representative. See also footnote 14.
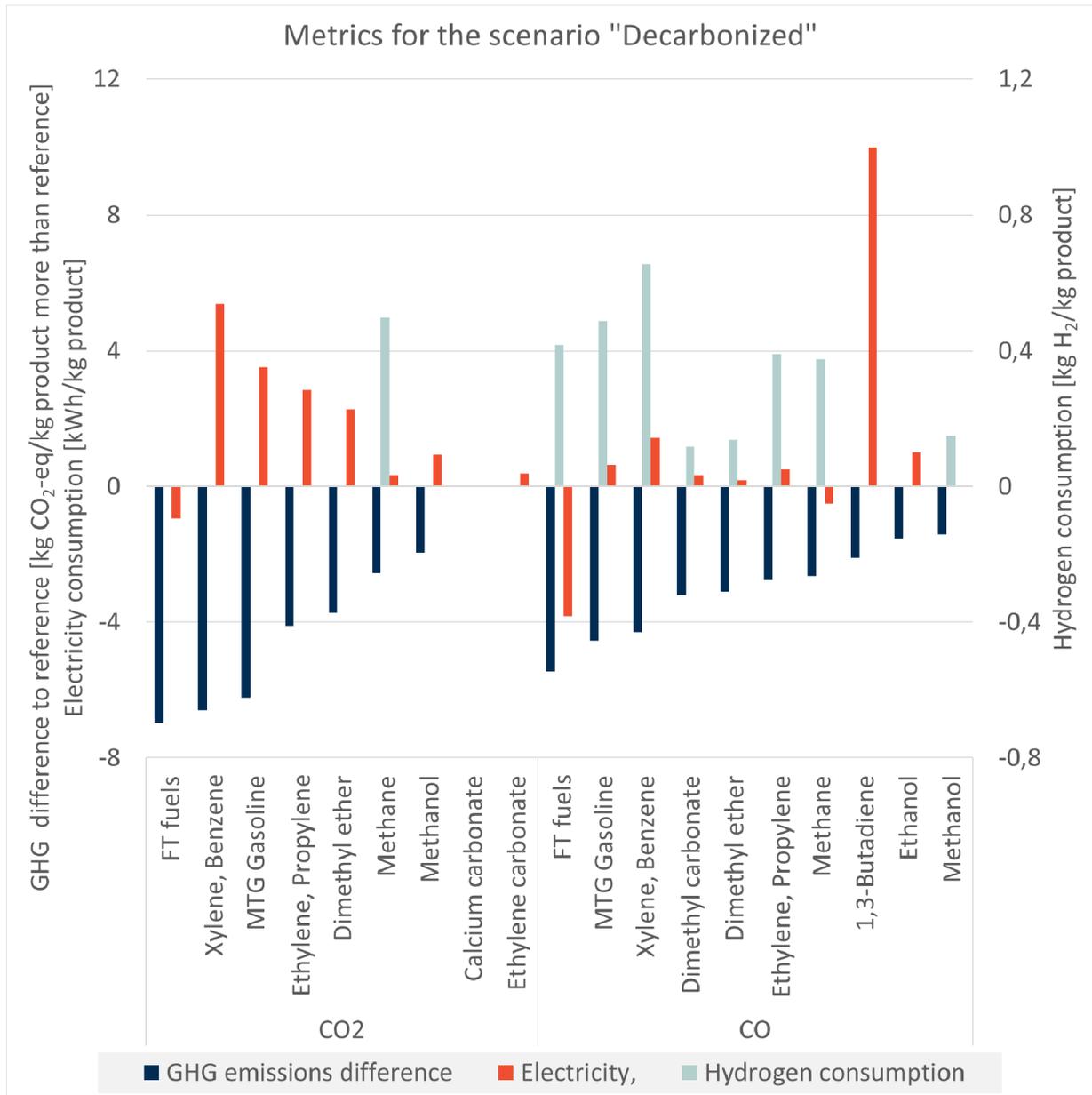
Figure 10: GHG difference, electricity and hydrogen consumption for all pathways. For CO_2 based pathways, the mean value for electricity and hydrogen consumption over all syngas routes is displayed for ease of reading.

Figure 11 shows the possible GHG savings per kWh of used electricity, if all the hydrogen is produced from electrolysis with a conversion efficiency of 50 kWh / kg hydrogen. As the FT process is a net producer of electricity[13], there is one syngas route from CO_2[14] where the whole pathway produces more electricity than it consumes, and thus no GHG emission reduction per kWh of consumed

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[13] The Fischer-Tropsch process is exothermic, and the heat is generally used to produce electricity.

[14] CO_2/steam reforming of fossil CH_4. In Figure 11 the fossil methane routes have been excluded.

electricity can be calculated. Besides FT fuels from CO_2, ethanol from CO as well as DME (from CO and CO_2) and dimethyl carbonate from CO have a high GHG reduction per kWh electricity in the best scenario and syngas route.
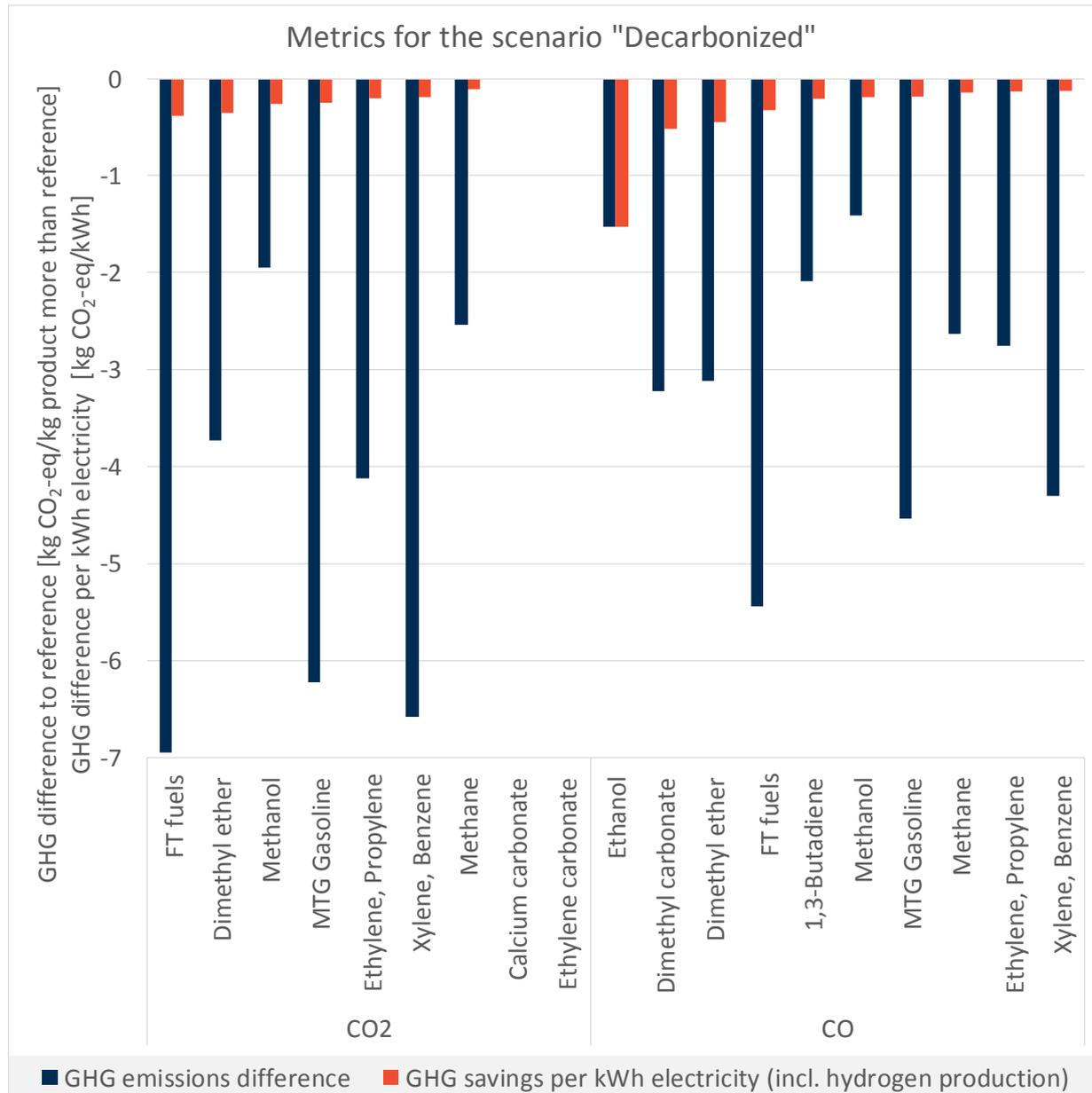
Figure 11: Possible GHG savings per kWh used electricity

Despite all uncertainties, all pathways are favourable regarding GHG reduction when using a decarbonized energy source.

The carbonates Calcium carbonate and Ethylene carbonate are already produced with CO_2. This is why no difference in GHG emissions is assumed to the reference process. In reality, there might be a reduction depending on the CO_2 source. Nevertheless, those processes do represent a potential CO_2 sink and should not be forgotten in the further analyses.

It is important to keep in mind that a big part of the GHG emissions is caused by the syngas production in nearly all pathways. A special focus should be put on the syngas production route and the CO/H_2 ratio needed for each product. In the figures above, the lowest consumption and highest emission reduction of all syngas routes is shown.

The current study simplified the environmental impact to GHG emissions and within that category to CO_2 for the core process, as data on other emissions are nearly impossible to obtain for the current state of the technologies. It is important to assess all environmental impacts going forward, especially if processes need special catalysts or create other emissions. One example is methane, which is a powerful GHG, so processes producing or using methane have to be analysed carefully to determine methane leakage.

5 Economic impacts

This chapter focuses on the key aspects of the economic assessment performed.

5.1 Impact of the main cost elements

The main cost elements included in the analysis are the CAPEX and OPEX costs. These are discussed in turn below.

5.1.1 CAPEX

The CAPEX is determined based on the processes needed to produce a given chemical for each pathway (i.e. the pathway is deconstructed into individual transformation reactions in the same manner as for the GHG assessment; see section 1.2). We have used conservative estimates for the CAPEX, based on current values, given that little variation is expected for these types of investment in the coming 15 years. Innovations and economies of scale could lead to lower costs, but small starting volumes and higher engineering costs could lead to cost increases.

CAPEX costs represent between 1 and 52% of the total costs included in the assessment, considering all pathways and scenarios. For certain pathways, such as methane (from CO or CO_2), CAPEX is almost negligible; while for others, such as ethanol from CO and FT fuels from CO_2, it is a major component in the analysis with over 20% of the costs in every scenario. In most cases, however, CAPEX is under 20%. Given its limited relative importance, CAPEX is not expected to be a decisive factor for decision making in most pathways.

For comparative purposes, the figure below shows the CAPEX compared to the OPEX. Since the CAPEX depends on the syngas routes (for the CO2-based pathways) and the OPEX depends on both the syngas routes and economic scenarios, the graph shows a minimum OPEX and minimum CAPEX and a range of OPEX and CAPEX per pathway showing the combination of all results (using the four economic scenarios and the four assessed syngas routes).
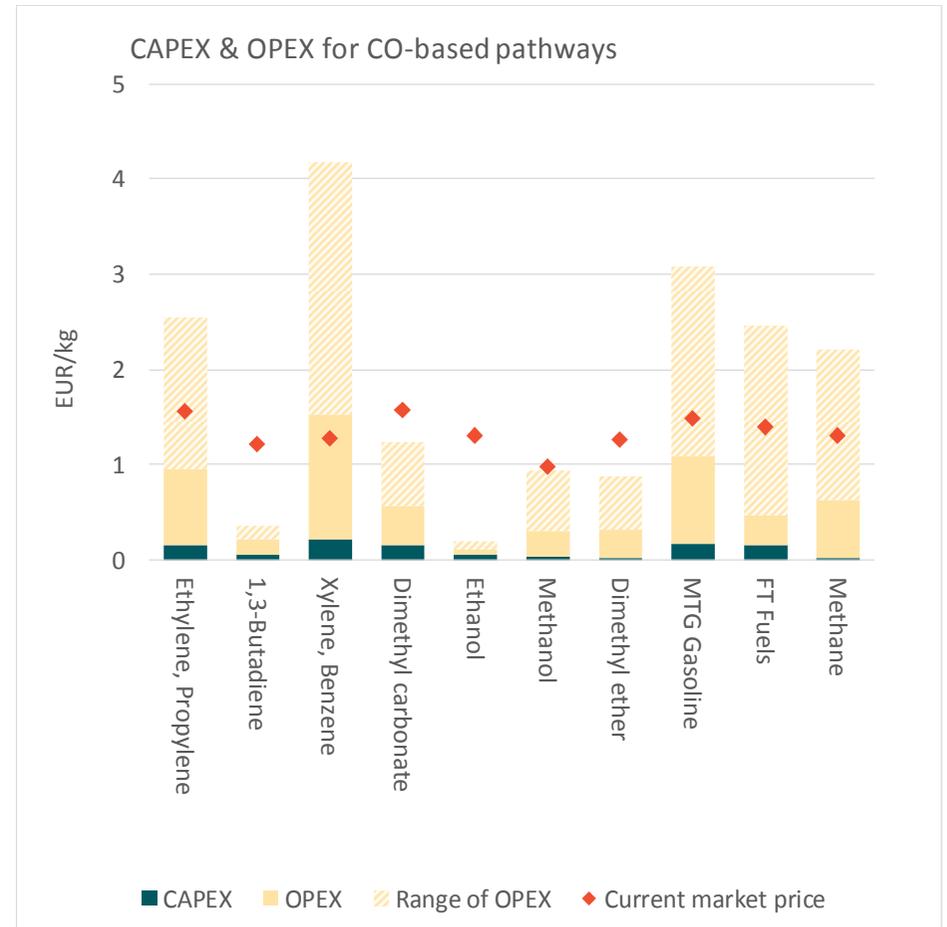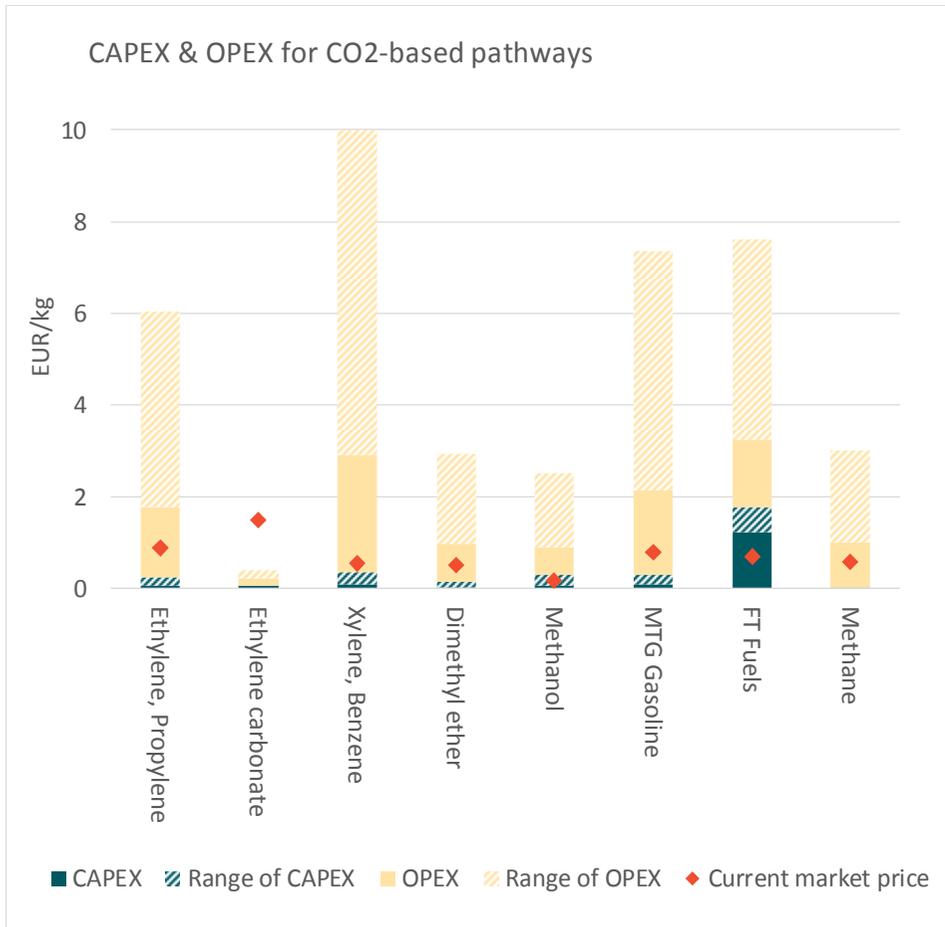
Unlike the range of OPEX and CAPEX costs, OPEX and CAPEX are not a range, the values of these two cost components are represented only by the upper side of the rectangle. The range of OPEX and CAPEX costs encompasses all possible combination under the scenarios and syngas routes. The CO-based pathways do not depend on the syngas routes; and hence the CAPEX does not vary.

Figure 12: CAPEX compared to OPEX costs for the different CO₂-based and CO-based pathways

The CAPEX is of relatively small importance in a CCU business case or investment decision. The investment amount is not that critical as long as the IRR (the Internal Rate of Return) is above the minimum required by the investor (for a specific level of risk). Especially with today's very low interest rates, the CAPEX is not a decisive factor in new CCU investments; the OPEX is.

5.1.2 OPEX

OPEX costs represent between 48 and 99% of the total costs included in the assessment, considering all pathways and scenarios. In this assessment, we have limited the OPEX costs to the following sub-components:

- Hydrogen costs
- Electricity costs
- Heat costs
- Carbon dioxide and carbon monoxide costs

These costs are directly linked to the material flow analysis set up in the GHG assessment, and therefore to the specific inputs required to carry out the processes. While these are not the only operational costs incurred, they do provide an adequate approximation. Other costs, such as those for catalysts, are more complex to estimate given the lack of information available in this respect. In several cases these OPEX components represent an income instead of a cost. This happens where, as part of the process, there is an output of heat or electricity. When this occurs, we have assumed that these outputs are sold at the same prices they are bought, according to the four scenarios introduced in section 1.3.

The figures below show the OPEX split per cost-component for CO_2-based pathways dependent on syngas under scenarios 1 and 4. Hydrogen costs make up the majority of OPEX for all CO_2-based pathways. Hydrogen costs are high if the pathways use syngas produced by reverse water gas shift (rWGS), compared to the high electricity costs when using syngas produced via HT SOC. Methane does not use syngas and therefore has the same OPEX, which consists mostly of hydrogen costs.

Costs are significantly lower under scenario 4 . about half of those under scenario 1. This is mainly due to the lower hydrogen price, but also to the positive effect of the lower electricity price. The CO_2-price plays a bigger role than under scenario 1, in relation to the other cost elements and also in absolute terms. Between the pathways and the syngas routes, we still see the same ranking as under scenario 1: ethylene carbonate is the cheapest, and benzene, xylene and MTG gasoline the most expensive.
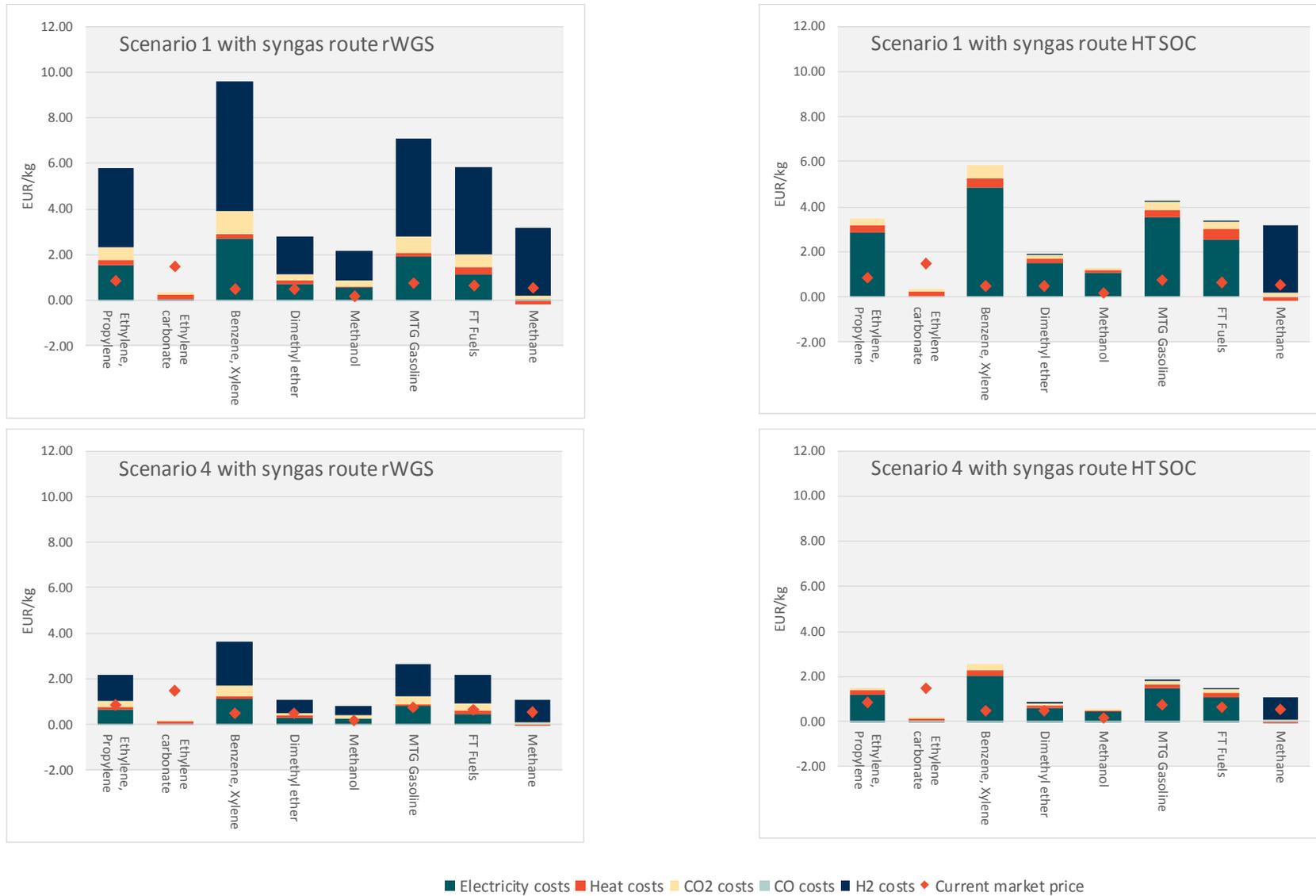
Figure 13: OPEX for CO₂-based pathways dependent on syngas under scenario 1 (high electricity and H₂ prices) and 4 (low electricity and H₂ prices)

For pathways using CO, the OPEX is significantly lower than for CO_2 based pathways. The largest OPEX cost component is hydrogen. Therefore, differences between scenario 1 and 4 are bigger for CO-based pathways: a change in hydrogen price from 6 ˮ/kg to 2 ˮ/kg leads to almost an equal drop in OPEX. On the other hand, lower electricity and heat prices lead to lower related income.
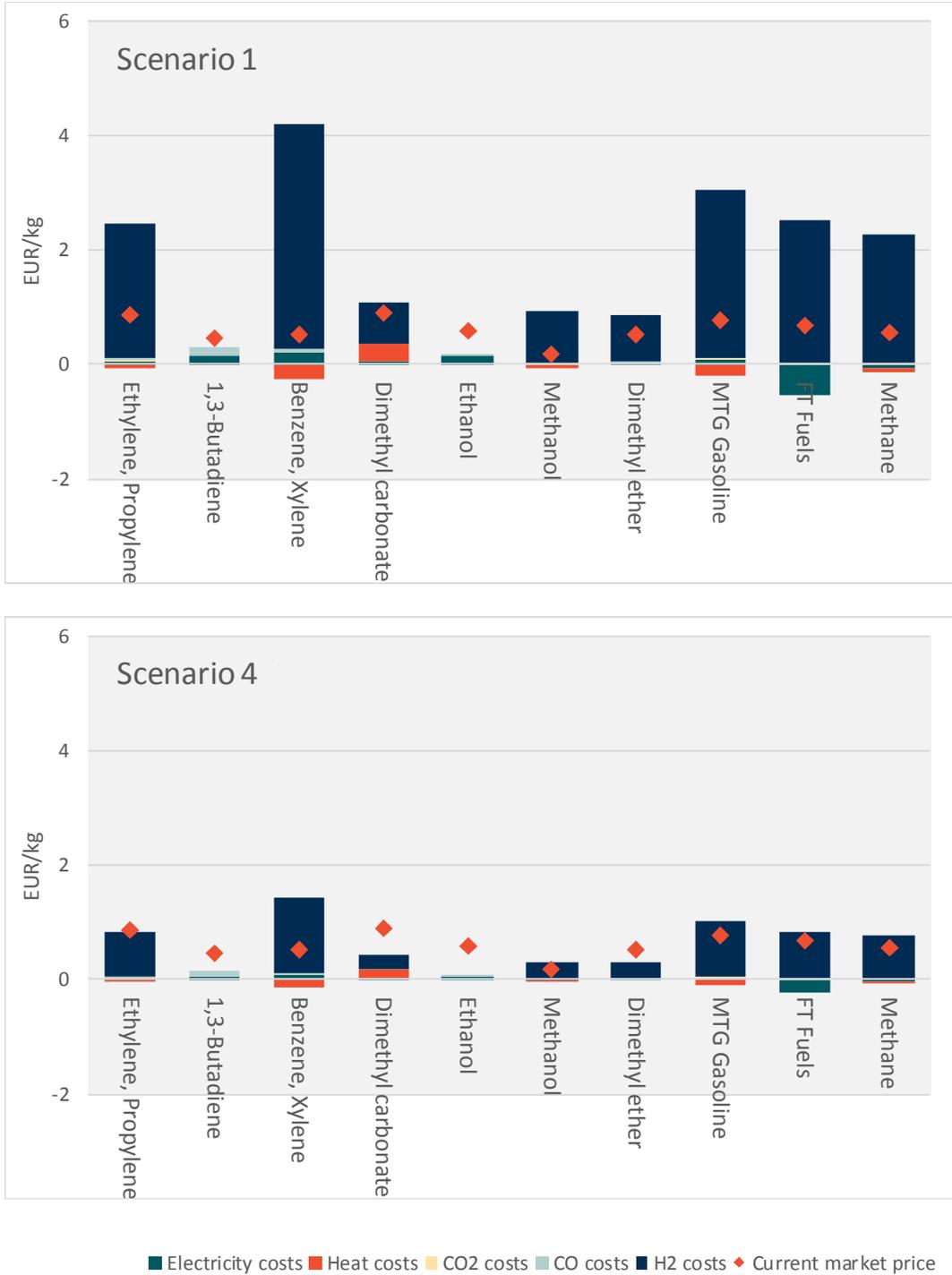
Figure 14: OPEX for CO-based pathways under scenario 1 (high electricity and H_2 prices) and 4 (low electricity and H_2 prices)

Overall, operational expenditures are crucial for CCU pathways and have a large impact on the business case. The future prices for the key inputs assessed can vary substantially due to a variety of factors (technical, fiscal, etc.) having a large impact on the business case. The accompanying Excel tool allows the user to use their own input prices and see their effect on the cost assessment.

Hydrogen cost

Only certain pathways require hydrogen and therefore have a hydrogen cost component. In those cases where hydrogen is an input to the process, it is the main cost component, representing over 30% of the total costs assessed (including CAPEX). There are many developments and uncertainties around hydrogen production and this can have a major impact on the business case. The use of 'green'(using renewable electricity) or 'blue'hydrogen (using natural gas and CCS) will also have an impact on hydrogen cost. Further, hydrogen can be used directly, which . depending on the demand . could impact price and availability.

Electricity cost

Electricity costs tend to be a large component of the calculated OPEX, either as an actual cost or as an income. For example, there is a surplus of electricity in the FT fuel and methane pathways from CO in every route and scenario, leading to an income for the business case. In contrast, for 1,3 Butadiene and Ethanol from CO, electricity is a major cost, ranging from 54 to 73% of the calculated costs.

Heat cost

Heat costs vary strongly per project, depending on the availability of residual heat from nearby industrial processes. However, not all pathways require heat, and in some cases, heat is generated as a result of the process. For example, 1,3 Butadiene, Ethanol, Dimethyl ether, and FT fuels from CO do not require heat in any route; while methane, ethylene, propylene, benzene, xylene, methanol and MTG gasoline pathways from CO generate heat in all their routes.

Carbon dioxide cost

The price for carbon dioxide has many elements that can vary per location and per project. These variables were extensively analysed in Deliverable 3.1. The CO_2 price projections included in the economic scenarios are based on the considerations presented in that deliverable. The CO_2 used depends on the chemical equations presented in section 4.1 and the different syngas routes based on the stoichiometry of the reactions. In general, syngas produced via reverse water gas shift is more sensitive to changes in CO_2 price than that produced via HT SOC. FT fuels have the highest share of CO_2 costs in relation to the total costs. These fuels are followed by CO_2 based compounds produced via the methanol to aromatics (MTA) (benzene and xylene) and methanol to olefins (MTO) (ethylene and propylene) reactions.

Carbon monoxide cost

The price of CO also depends on many elements which were assessed in Deliverable 3.1. Currently, as analysed in Deliverable 1, the main source for CO (volume-wise) is the steel industry. To date,

most of this CO is combusted to produce heat or electricity to avoid releasing toxic CO. The following are key elements for the price of the CO:

- The opportunity cost for the heat or electricity currently produced.
- The capture cost and degree of purity required[15] (though there is limited experience and research on this).
- The ETS coverage, as CO_2 released as a result of the CO combustion is part of the ETS but the ETS framework for processing CO is unclear.

1,3 Butadiene (4C4) is the product most affected by the cost of CO in relation to the overall costs. Under the most favourable scenario (scenario 1), the OPEX costs for 1,3 Butadiene are only made up of CO (~ 56 %) and electricity (~ 44%) costs. Under the least favourable scenario (scenario 4), the low electricity price makes the cost of CO more prevalent in relation to the overall cost. As seen from

■ Electricity costs ■ Heat costs ■ CO2 costs ■ CO costs ■ H2 costs ◆ Current market price

Figure 14, in all other cases, CO costs constitute a very small component of overall OPEX.

5.2 Most financially competitive pathways

5.2.1 Most competitive pathways for CO_2-based products

This section focuses on the four most competitive pathways for CO_2-based products compared to current market prices (i.e. the most competitive pathways). Ethylene carbonate is the only pathway with costs below the current market price. This is likely due to the fact that the CCU-pathway is the same as the conventional process[16] but marginal costs and the costs of a catalyst are not included in our assessment. The other pathways whose production costs are closest to current market price are:

- Dimethyl ether (DME)
- Methane
- Methanol

The figure below shows these four pathways, using reverse water gas shift syngas route, across the four assessed economic scenarios. Scenario 1 is overall the least favourable, while scenario 4 is the most favourable one, leading to the lowest operational costs. The favourable effect is mostly due to

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[15] CO from steel production is mixed with a variety of other elements, volume-wise mainly N_2 and CO_2 but also heavy metals or other pollutants.

[16] Ethylene Carbonate process patent: US4233221A

lower hydrogen costs, hence the impact is limited for pathways (such as ethylene carbonate) which do not require hydrogen.
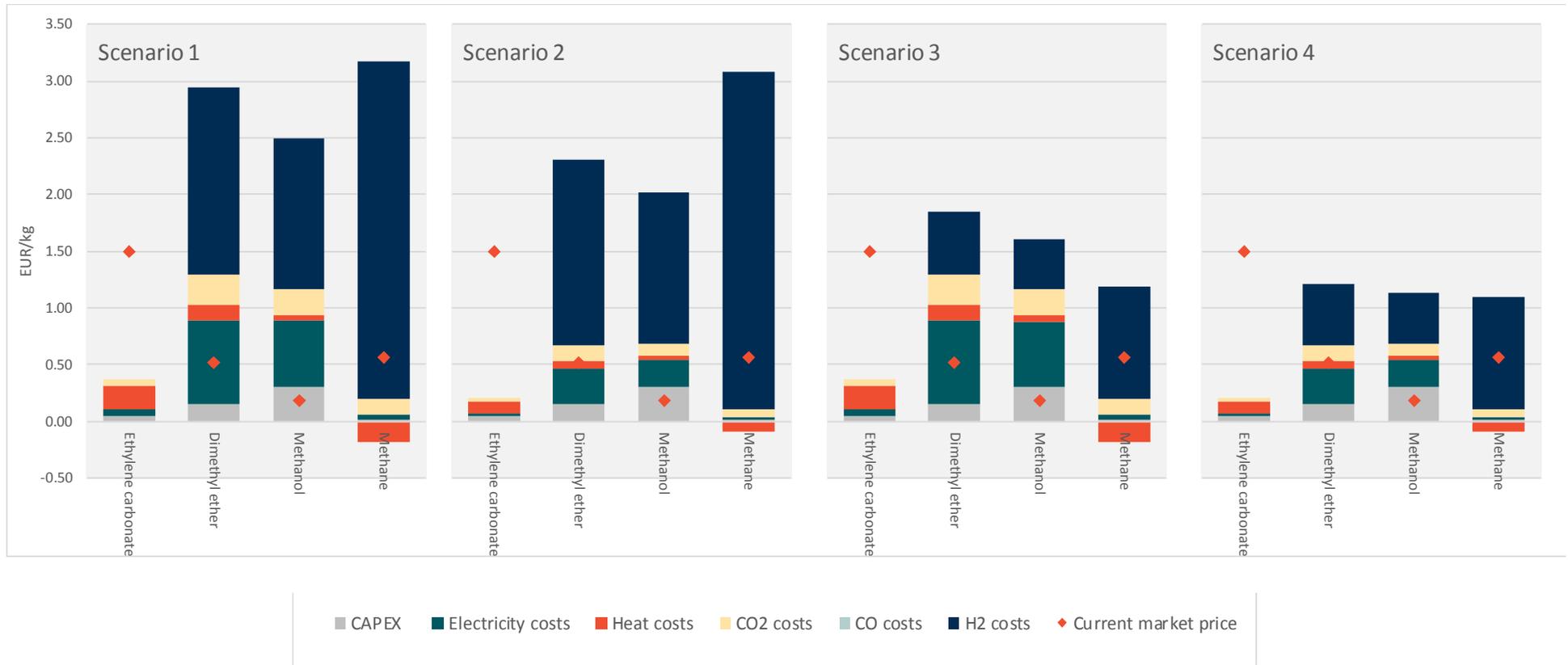
Figure 15: Assessed costs for CO₂-based pathways closest to market prices (Reverse Water Gas Shift route for syngas production)
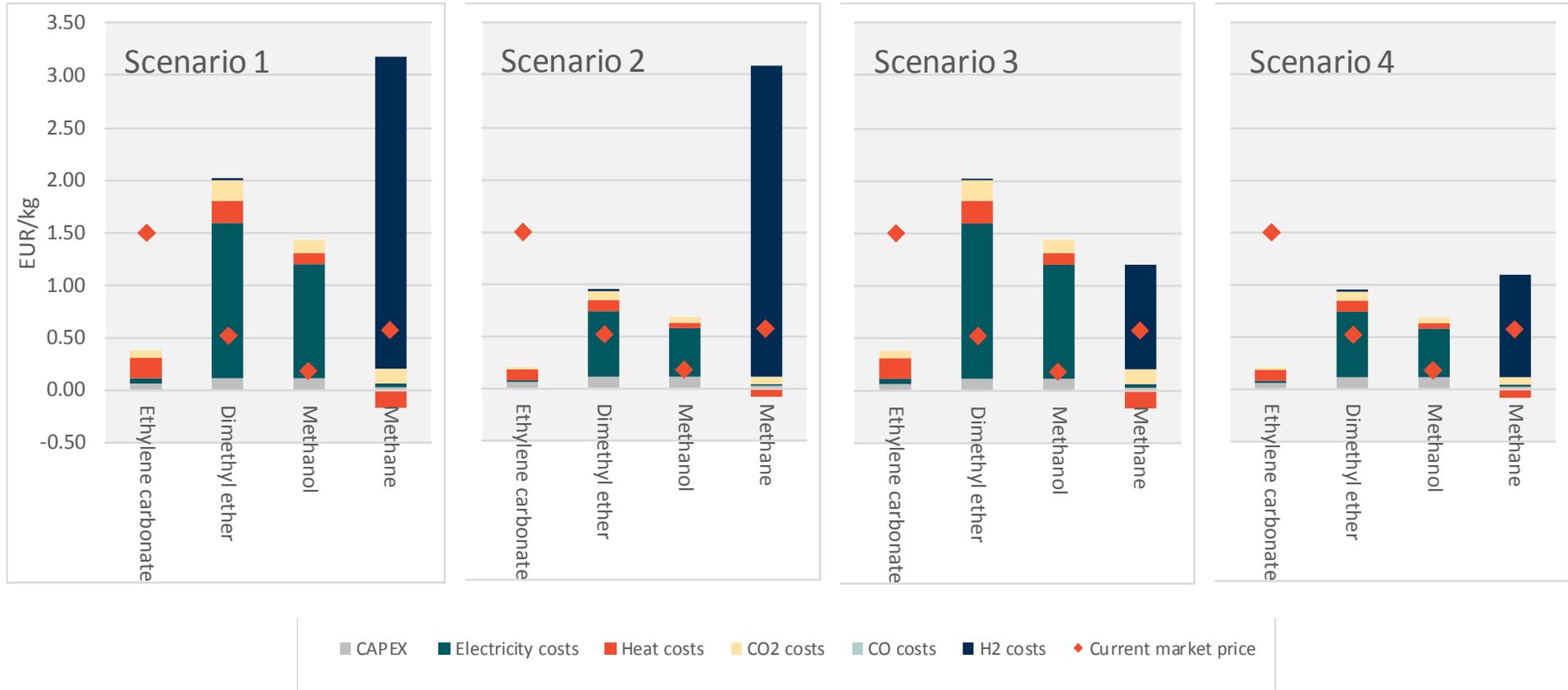
Figure 16: Assessed costs for CO$_2$-based pathways closest to market prices (HT SOC route for syngas production)

Using the HT SOC syngas route instead of reverse water gas shift, the production costs change for dimethyl ether (DME) and methanol. The other two pathways, ethylene carbonate and methane, are not dependent on syngas. Although rWGS uses hydrogen and more CO_2, it uses less electricity and heat than HT SOC. Production costs of DME and methanol produced via HT SOC depend mostly on electricity prices, and via rWGS on hydrogen prices. Overall, the advantages of a lower CAPEX and no hydrogen costs make these pathways cheaper when HT SOC is used.

Ethylene carbonate

As mentioned above, the fact that the calculated costs of producing ethylene carbonate are below the current market price is likely due to excluding profits, marginal and catalyst costs from the analysis. Ethylene carbonate is H_2 and CO-independent. Hence, the cost of this product is the same under scenarios 1 and 3 on the one hand, and 2 and 4 in the other hand. Ethylene carbonate is mostly affected by heat costs. Therefore, scenario 2 and 4 are the most favourable for this pathway.

Dimethyl ether (DME)

In the best case (based on scenario 4 and the HT SOC syngas route), the production of DME from CO_2 is 79% more expensive than the current market price. DME production costs via HT SOC stem almost entirely from electricity costs, whereas the costs of DME production via reverse water gas shift are based on both H_2 costs and electricity costs. Scenarios 3 and 4 with a low hydrogen price therefore make the production costs considerably lower.

Methanol

The production of methanol is also dependent on syngas. In the best case (based on scenario 4 and the HT SOC syngas route), the production costs of methanol are 267% above current market prices. The reverse water gas shift route makes the production costs at least 504% more expensive than current market prices.

The scenarios affect the production costs of methanol in a similar manner as those of DME. The composition of the production costs is somewhat similar in both pathways: both depend on hydrogen (except when using the HT SOC route), electricity and CO_2. However, methanol has a higher CAPEX and lower OPEX than DME. Therefore, the production costs are less affected by the different scenarios than those of DME. But they still have a big impact: for DME, methanol and methane, production costs are more than twice as high in scenario 1 as in scenario 4, regardless of the syngas route of choice.

Methane

Methane from CO_2 is produced via the Sabatier reaction which involves the methanation of carbon dioxide and is not dependent on syngas. Methane produced by CCU is over 2.5 times more expensive than the current market price in the best-case scenario (scenario 4). Under all four scenarios the major cost component for methane production is the cost of H_2. Thus, it is not surprising that the overall costs are highest for those scenarios in which H_2 prices are high (scenario 1 and 2).

## 5.2.2 Most competitive pathways for CO-based products

This section focuses on the four most competitive pathways for CO-based products compared to current market prices (i.e. the most competitive pathways). As highlighted in section 4.2.2 on the economic assessment overview, CO-based pathways have lower overall costs than the CO_2-based pathways. This is not surprising since thermodynamically CO_2 is a more stable, less reactive molecule and thus requires more energy to be activated.

Based on this, the assessed production costs of ethanol and 1,3-butadiene from CO are lower than the current market price for these products. However, as in the case of ethylene carbonate produced from CO_2, this is likely due to the fact that marginal costs and the costs of catalysis have been excluded from the analysis. Next to 1,3-butadiene and ethanol, CO-based pathways where the cost of production is close to the current market price are:

- Dimethyl carbonate
- Dimethyl ether

These four pathways are closest to current market prices in scenarios 1, 2 and 4. Only in scenario 3, with high electricity prices and low hydrogen costs, the production of gasoline and diesel is closer to market prices than dimethyl carbonate. This is because these two pathways have negative costs for electricity.

The figure below shows the four pathways across the four scenarios. Scenario 4 (with low electricity, heat and hydrogen costs) is the most favourable one, leading to the lowest operational costs.
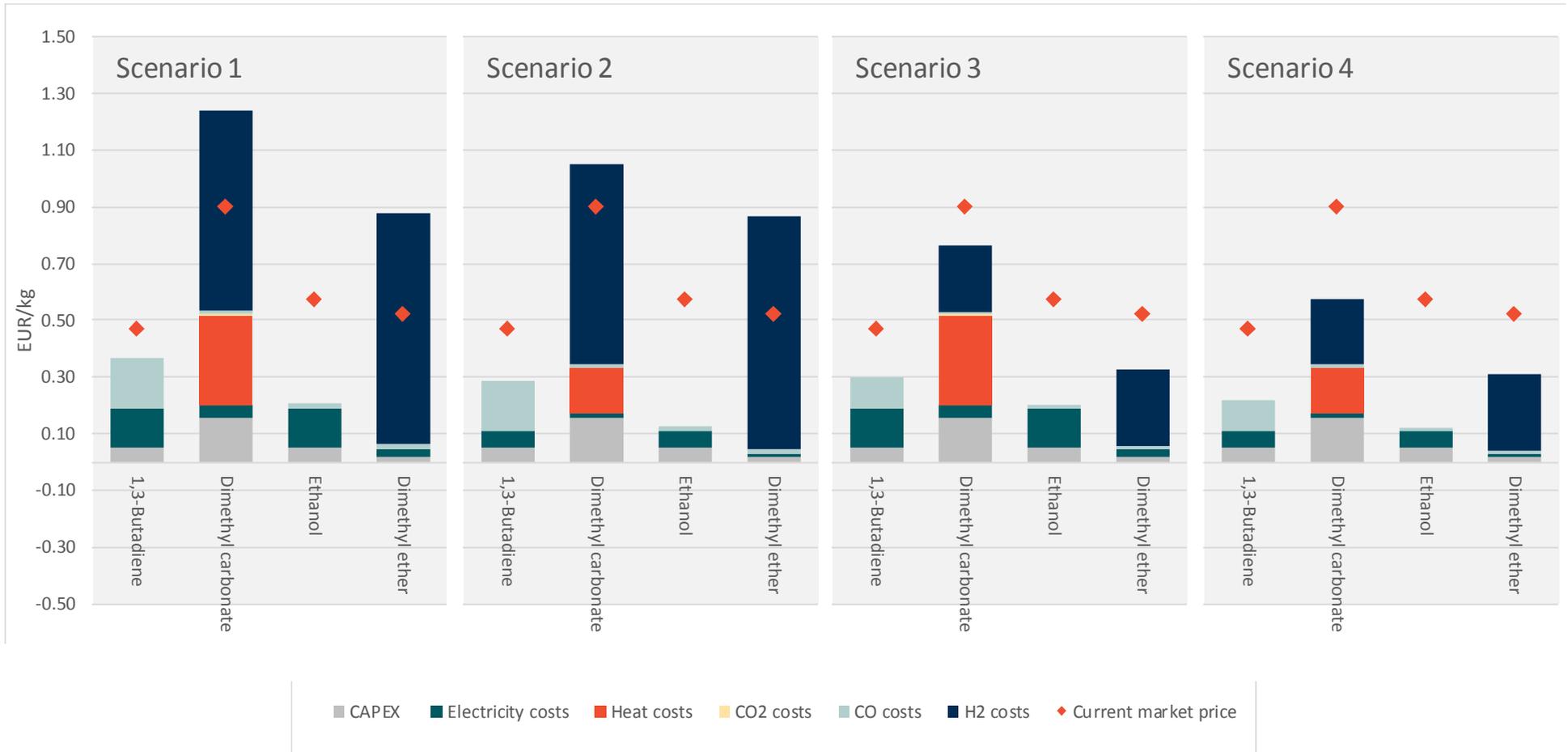
Figure 17: CO-based pathways closest to market prices in the four scenarios

1,3-butadiene and ethanol

Both ethanol and 1,3-butadiene from CO are produced via the gas fermentation of carbon monoxide by the anaerobic bacterium Clostridium. Both pathways are independent of CO_2 and H_2. In the case of 1,3-butadiene, the CO price, electricity price and CAPEX constitute the totality of the final cost under all scenarios, with CO price being the largest cost component under scenarios 1, 2 and 4 and electricity being most important component under scenario 3. In the case of ethanol, electricity and CAPEX are the major cost components under all scenarios with CO price representing a very small part of the total costs. For both 1,3 butadiene and ethanol, scenario 4 is the most favourable, with production costs being an estimated 46% and 21% of current market prices respectively. This can be ascribed to the low electricity price and low CO capture cost.

Dimethyl carbonate

Dimethyl carbonate is produced via the carbonylation of methanol in the presence of oxygen. Under scenarios 1 and 2, the costs of producing dimethyl carbonate by this pathway are higher than the current market price. However, under scenarios 3 and 4, this way of producing the chemical is cheaper than the current market price. This is thanks to the lower hydrogen price, which makes up the majority of the production costs.

Dimethyl ether (DME)

The costs of dimethyl ether made from carbon monoxide are largely driven by H_2 prices under all scenarios. Under scenario 1 and 2 the high hydrogen prices make the costs of production significantly higher than the current market price of the product. The lower H_2 prices under scenario 3 and 4 would make the production of dimethyl ether from CO economically viable, with production costs lower than the current market price.

5.3 Sensitivity analysis on electricity prices

High levels of intermittent electricity production are expected to create a demand for storage and/or moments with very low electricity market prices. Therefore, in many discussions, electricity costs for CCU are deemed very low. However, these low electricity prices are incidental, and would affect the CAPEX costs, as it would limit duration of operations (not 24/7). To assess this potential outcome, we have made a sensitivity analysis considering electricity prices at zero, along with a 20% utilisation rate of the installations (which equals to a five-fold increase of the CAPEX costs in the assessment).

When there are no electricity costs (but utilisation remains at 100%), several additional pathways become competitive under the most beneficial economic scenario (scenario 4) when using the solid oxide cell syngas route. However, when we account for the increased CAPEX costs due to lower utilisation rates, this is no longer true (see figure below). Already x3 CAPEX leads to higher costs than current market price for most pathways, except for ethylene carbonate (which is also under current

market price in the reference), as well as 4 CO-based pathways: 1,3 butadiene, dimethyl carbonate, DME, and ethanol.
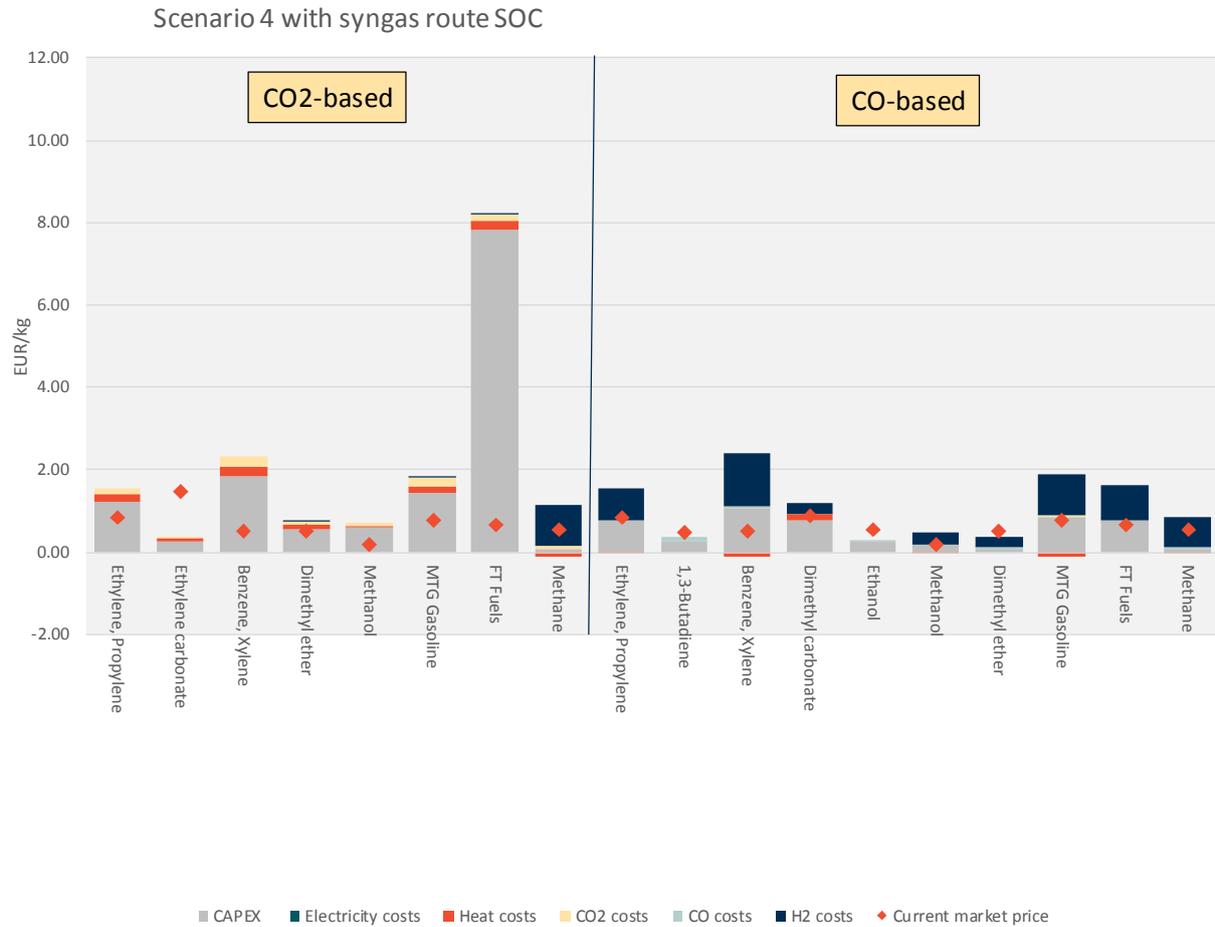
Figure 18: Assessment assuming electricity prices are 0 and CAPEX is 5x higher (using most beneficial economic scenario, scenario 4 and SOC syngas route)

5.4 Conclusions and considerations regarding the CCU business case

Conclusions

Although we expect a broad *technical* potential for CCU products to be available by 2030, the current framework conditions and price expectations do **not allow for profitable business cases** in the vast majority of the CCU routes investigated.

Overall, the products made from CO have a better economic outlook; even with the current uncertainties on CO capture prices. On the other hand, in almost all scenarios the production of fuels like gasoline and diesel (from CO or CO_2) are among the costliest due to the high hydrogen price penalty.

The main barriers for a profitable business case are:

- the **high cost for the additional energy** required to turn the CO_2 into more valuable products; and

- the high **cost for hydrogen** (if required) to make hydrocarbons/fuels.

The cost for the capture and transport of CO_2, on the other hand, have a limited impact compared to other cost elements.

High levels of intermittent electricity and related low electricity prices will have an impact in the business case. However, these low prices are incidental and would not be sufficient to make CCU profitable in the short to medium term. If CCU is to be used for energy storage, i.e. if CCU production processes are only operational during the hours of an electricity surplus, the business case will considerably deteriorate as 24/7 operations are no longer possible, leading to higher CAPEX per kg of product and increasing overall costs. Further, given market dynamics and the fact that these very low market prices are based on incidental moments only, it is expected that once an alternative demand for electricity is introduced (e.g. for CCU), prices will increase.

Considerations

Results may differ depending on the specific projects and locations. This section provides a short list of the considerations taken within our assessment.

Focus on large market products (volume-wise): The assessment presented has not taken into account smaller markets nor high-end products or consumers who are willing to pay higher prices for CO_2-neutral products. We have specifically selected products which have a large market volume. There may be CO or CO_2 based products which may have better economic outlooks, but which are not substantial in terms of CO or CO_2 utilised.

Economic benefits of mineralisation: Mineralisation (concrete/bricks) is not in the scope for this analysis; however, it has two major economic advantages over CCU in the chemical industry. Firstly, the chances for inclusion of these type of products under the ETS are much higher (because it entails permanent storage) and, secondly, the energy costs are much lower (because it involves an exothermic reaction). Further research in this area should be encouraged.

Use of assumptions due to uncertainty: Our analysis is based on a large number of assumptions due to the current state of knowledge and limited industrial activities in the sector. The assumptions used to define the four economic scenarios are not meant to predict the future, but rather to provide a range of potential directions in which key parameters will go in the future. Therefore, the outcomes of the economic assessment are meant to give an indication of the major sensitivities and allow for comparing the different pathways rather than providing absolute numbers. The excel tool developed gives the reader the opportunity to introduce their own assumptions and assess the corresponding results.

Limited impact of CO_2 costs and potential effect of ETS: Currently, CO_2 capture and transport costs have a limited impact in the cost assessment. However, the inclusion of CCU pathways under the ETS could improve the business case depending on how this was regulated. There would be a

positive impact on the business case if the full amount of CO_2 included in the product would be allowed under the ETS, as there would be a perceived benefit for each ton of CO_2 utilised. However, we assume this is only likely for mineralisation (permanent storage).

Impact of CCS: If CCS is in place, CO_2 would become more easily and likely more cheaply available for CCU. However, this would hardly impact the economics for CCU as, in order to obtain CO_2 from a CCS operator (instead of storing it), a payment at least as high as ETS price they receive for permanent storage would be required. Therefore, a higher ETS price would make CCS the preferred option (compared to CCU).

6 Outlook

This report presented the technical details of the economic and environmental analyses of the selected pathways. Aggregated results and an overall conclusion of the project results will be presented in deliverable 4.4.

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8 Table of figures

9 Annex A: CAPEX estimates and sources

The table below summarizes the CAPEX estimates and the sources from which these were derived.

*Note: The capex for steam and dry methane reforming are expected to be comparable. We use the value reported by Jarvis (0,027 " /kg) et al. for both processes.

Table 4 CAPEX estimates and sources

Process	CAPEX (Ö/kg)	Reference
Methanol-to-Olefines (MTO)	0,06	Assumes that the CAPEX is the same for MTO, MTA and MTG processes, see discussion below.
Methanol-to-Aromatics (MTA)	0,06	"Methanol to Aromatics" 2016, Ward el al. University of Wyoming, Undergraduate Honours Thesis
Methanol-to-Gasoline (MTG)	0,06	Assumes that the CAPEX is the same for MTO, MTA and MTG processes, see discussion below.
Dimethyl ether from syngas	0,019	"Chemical Engineering Design I Final Report", 2014, Alsharif Aliyev, Ataki iyev and Rustamov, Middle East Technical University[17]
Water-Gas-Shift (WGS)	0,005	"Design, Optimization, and Control of Membrane Reactor for Water-Gas Shift Reaction", 2017, Saw Shuey Zi, Curtin University, Doctoral Thesis.[18]
Reverse Water-Gas-Shift (RWGS)	0,036	Dimitriou *et al.* "Carbon dioxide utilisation for production of transport fuels: process and economic analysis" Energy Envirion Sci., 2015, 8,1775
High Temperature Solid Oxide Cell (HT SOC)	0,072	"Syngas production via high-temperature steam/CO_2 co-electrolysis: an economic assessment", FU *et al.* 2010
Methanol from syngas via	0,149	"Technoeconomic Assessment of Methanol Synthesis via CO2

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[17] https://www.slideshare.net/JozephAlsharif/dme-plant-project-final-report

[18] https://espace.curtin.edu.au/bitstream/handle/20.500.11937/59694/Saw%20S%202017.pdf?sequence=1

Process	CAPEX ($€/kg$)	Reference
hydrogenation		hydrogenation" Michailos, Amstrong, Styring Shared in confidence, not yet published
Methanol via Sorption Enhanced Water-Gas-Shift (SEWGS)	0,026	CORESYM 2017
Dry reforming	0,027	Jarvis, S.M.; Samsatli, S; "Technologies and infrastructures underpinning future CO_2 value chains" A comprehensive review and comparative analysis", Renewable and Sustainable Energy Reviews 85 (2018) 46-68
Sabatier	0,019	Jarvis, S.M.; Samsatli, S; "Technologies and infrastructures underpinning future CO_2 value chains" A comprehensive review and comparative analysis", Renewable and Sustainable Energy Reviews 85 (2018) 46-68
Fischer-Tropsch reaction	0,153	Jarvis, S.M.; Samsatli, S; "Technologies and infrastructures underpinning future CO_2 value chains" A comprehensive review and comparative analysis", Renewable and Sustainable Energy Reviews 85 (2018) 46-68
Ethanol via fermentation	0,051	Saud, MSc. Thesis "Profitability of Ethanol Production by Gas Fermentation from Steel Mill Flue Gases"
Carbonylation with O2	0,128	de Groot *et al.* "The Industrial Production of Dimethyl Carbonate from Methanol and CO_2"
Ethylene carbonate production	0,03	https://ihsmarkit.com/products/chemical-technology-pep-reviews-ethylene-carbonate-from-ethylene-2003.html

10 Annex B: Product classification and description

Figure 19 contains a grouped list of the products that are analysed, with the mention if it can be produced from CO or CO_2 or both and a short description where they are most used.

Figure 19: List of analysed products and their use

11 Annex C: Market Prices of products not found in PRODCOM

Product	EUR/ton	Source
Dimethyl ether	521	Avg Jan 2011/ Mar 2018 for CEIC data[19]
Calcium carbonate	152	Average of existing prices available from Indianexim resources[20]
Dimethyl carbonate	900	Average from different sources[21]
Ethylene carbonate	1500	Average from source[22]

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[19] https://www.ceicdata.com/en/china/china-petroleum--chemical-industry-association-petrochemical-price organic-chemical-material/cn-market-price-monthly-avg-organic-chemical-material-dimethyl-ether-990-or-above

[20] http://www.indian-exim.com/prices/ch_inorganic.htm

[21] https://www.made-in-china.com/price/dimethyl-carbonate-price.html and https://www.lookchem.com/product_Competitive-price-professional-manufacturer-for-Ruifeng-Dimethyl-carbonate-/13966131.html

[22] https://www.made-in-china.com/products-search/hot-china-products/Ethylene_Carbonate_Price.html

12 Annex D: Life Cycle Inventory sources

The sources (Peppel 1958; Raines and Ainsworth 1980; Choudhary and Rajput 1996; Keil 1999b; Vaswani 2000; Clausen *et al.* 2010; Eloneva *et al.* 2012; Becker *et al.* 2012; Trippe *et al.* 2013; Xiang *et al.* 2014; Pérez-Fortes *et al.* 2014; Assen *et al.* 2015; Kongpanna *et al.* 2015; Giglio *et al.* 2015; Handler *et al.* 2016; Garcia-Herrero *et al.* 2016; Hannula 2016; Sternberg and Bardow 2016; Wernet *et al.* 2016; Bazzanella and Ausfelder 2017; Collet *et al.* 2017; Hoppe *et al.* 2018; 2018; Jones and Zhu; Zi) have been used to build the input-output lists of the sub-processes. Please refer to the accompanying Excel tool for details on which source was used for which process.