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 *4.2*:
Methodology to assess the environmental impact and energy efficiency of CCU

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1. Introduction

This deliverable presents the framework and methodology to assess the CO/CO_2 resources and the utilization pathways identified in Work Package 2. The aim is to provide a comparative energetic and environmental analysis of the different pathways.

Carbon(dioxide) Capture and Utilization (CCU) is a growing and broad field of research, which poses various challenges for life cycle assessment (LCA) methods – this is valid for the CO utilization as well. First of all, most technologies in early stages of development are afflicted with uncertainties about technological choices and advances, but also lock-ins (Lock-in effects occur when a technological choice influences other choices in the future, especially if large infrastructure is needed, an example could be urban planning for cars, which would make it extremely difficult to switch to a public transport concept later on.) Similar to other chemical production technologies, they need to be highly integrated to be energy and cost efficient, and therefore have the advantage but also risk of synergies between processes. Secondly, CO and CO_2 utilization processes when producing chemicals or fuels generally have high electrical energy consumption, replacing the energy contained in fossil inputs of conventional pathways, so the electricity mix plays a predominant role. It has been found over and over again that most CCU technologies only emit less greenhouse gases (GHG) if the electricity mix contains a high percentage of renewables. Another debated point is the use of CO_2 as a raw material and how to account for it under different capture scenarios. LCAs for CO/CO_2 utilization are therefore labour-intense and need a good understanding of LCA methodology and chemical process engineering.

Different initiatives are working on harmonizing LCAs for CO/CO_2 utilization (e.g. the soon to be published "Guideline for Life Cycle Assessment of CO_2 utilization [1]). This will help making results comparable and easier to re-use. For now, methodologies are not harmonised. Hence, a general comparison of different LCA results is not fully meaningful.

For this reason, this study proposes an LCA screening and a harmonization by using common scenarios for the most important inputs, based on the aforementioned study [1].

It is important to clarify that this deliverable will focus only on LCA screening which accounts for environmental impacts. Other issues such as technical feasibility, potential CO/CO_2 uptake and economic impacts are addressed by other deliverables under the CarbonNext project:

- Deliverable 1.1 highlights the availability of CO/CO_2 sources and characterises them
- Deliverable 2.3 defines the CO/CO_2 utilization pathways to be assessed with this methodology, including their technical feasibility
- Deliverable 3.1 analyses at what market conditions it becomes attractive to capture and transport CO/CO_2, which can be used for further processing
- Deliverable 4.1 provides the methodology to assess the business case of the CO/CO_2 utilization pathways.

This deliverable first defines the scope of the CCU LCA screening and provides a general framework for the methodology. Then, it defines three scenarios for the generation of inputs (hydrogen, heat and electricity) and related assumptions which have an impact on the assessment. Finally, the methodology which will be used to assess each of the CO/CO_2 utilization pathways is described.

2. Life Cycle Assessment Framework

ISO 14040 [2] defines the general framework for LCA studies as shown in Figure 1. It defines the steps and interactions in conducting a life cycle assessment to determine environmental impacts of a product or service. The main steps are:

- Goal and scope definition: clearly defining the goal, knowing that this influences the choice of methodology, the quality of the data needed and also the scope and reference processes. A clear scope avoids neglecting parts of the life cycle.
- Inventory analysis: finding and gathering the right data in sufficient quality is a challenge, especially for new technologies. Sources, uncertainties and assumptions must be documented.
- Impact assessment: In this step, relevant impacts on the environment are extracted from the inventory analysis. All relevant impacts should be looked at.
- Interpretation: Every step needs an interpretation activity, to check the results against the goal and scope and adapt the work if necessary.

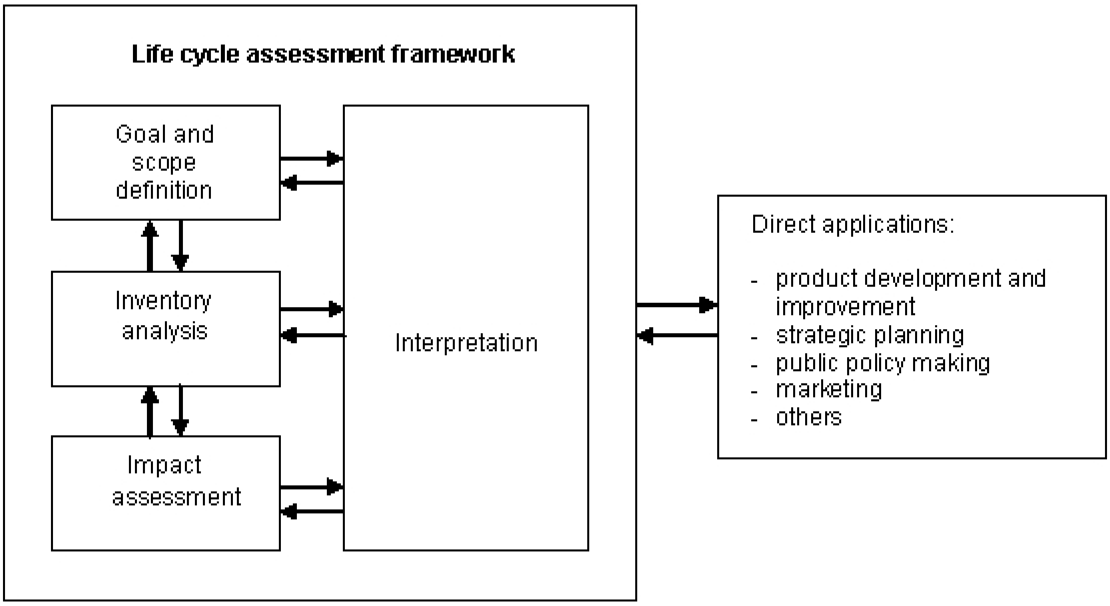


Figure 1: Phases of an LCA according to ISO 14040

As a first indicator of environmental performance for technologies with low TRL and no special “hot spot” emissions, climate change is generally used for CCU pathways. In this case, ISO/TS 14067 [3] and guidance in [4] can be followed, which define the carbon footprint of products very close to ISO 14040, but limited to the impact “climate change”.

As this is a screening study and analysis of existing gaps, we will follow the ISO/TS 14067 framework as much as the scope and goals of this study allow. A screening of available data showed that uncertainties and data availability make it difficult to look at other environmental impacts beyond climate change in the scope of this study.

3. Goal and scope definition

3.1 Goal

The goal of the study is to compare the selected routes from deliverable 2.3 in terms of GHG emissions. To eliminate pathways that are not energy efficient, a screening study will be conducted. All pathways will be compared with each other and with their respective conventional route.

Energy efficiency is defined relative to other CO/CO_2 utilization pathways yielding the same product. For instance, four methanol production pathways are considered from CO_2. Energy efficiency is an important criterion to select the best way to produce methanol.

Carbon efficiency is defined relative to the conventional pathway yielding the same product. For instance, if methanol produced from CO_2 has higher GHG emissions than the conventional route (using the same electricity mix, heat and hydrogen production), then the CCU pathway is not carbon efficient.

3.2 Scope

As the purpose of the CO/CO_2 utilization products is to replace a conventionally produced product, the analysis can be limited to a cradle-to-gate analysis. This means that only the production of the product is compared. Product combustion and characteristics, use as well as end-of-life phase are considered to be identical.

As this is a screening study, the main focus is on the main energy and material inputs. All smaller inputs, especially catalysts, but also plant lifecycle, will be mentioned, but it is outside the scope of this study to include a detailed LCA on them. This is deemed acceptable as the quantities of those inputs are very low. Nonetheless, they might have important environmental impacts as some of them include rare metals or complicated production steps. This should be included in a further analysis if a particular pathway is to be considered for deployment.

In all cases, this study does not produce comprehensive LCAs. LCAs are product and location specific. Therefore, whilst this approach of screening can be used to eliminate the most inefficient pathways it cannot replace a full LCA. A full LCA, not just carbon footprinting, would need to be carried out to draw conclusions on deploying a specific pathway in a specific circumstance. However, this LCA would be carried out at a much later stage and in the first instance a screening will give the desired outcomes to enable selection between pathways.

3.3 Multi-functionality

Some CCU pathways may be embedded in sophisticated further processes and thus a noticeable number of by-products are cross-linked. This is the case for the gas fermentation pathway producing 1,3-butadiene, which currently produces about ten times more ethanol than 1,3-butadiene. The gasoline production via the methanol-to-gasoline process also produces a sizeable amount of LPG (liquefied petroleum gas) as a by-product.

Those multi-functional pathways will be treated with a system expansion. Instead of comparing just the main product with the conventional product, the functional unit will be the whole output of the CCU process. So e.g. for gasoline, the functional unit will be “1 kg of gasoline + 0.26 kg of LPG”. This will be compared to producing the same amount of gasoline and LPG via the conventional route.

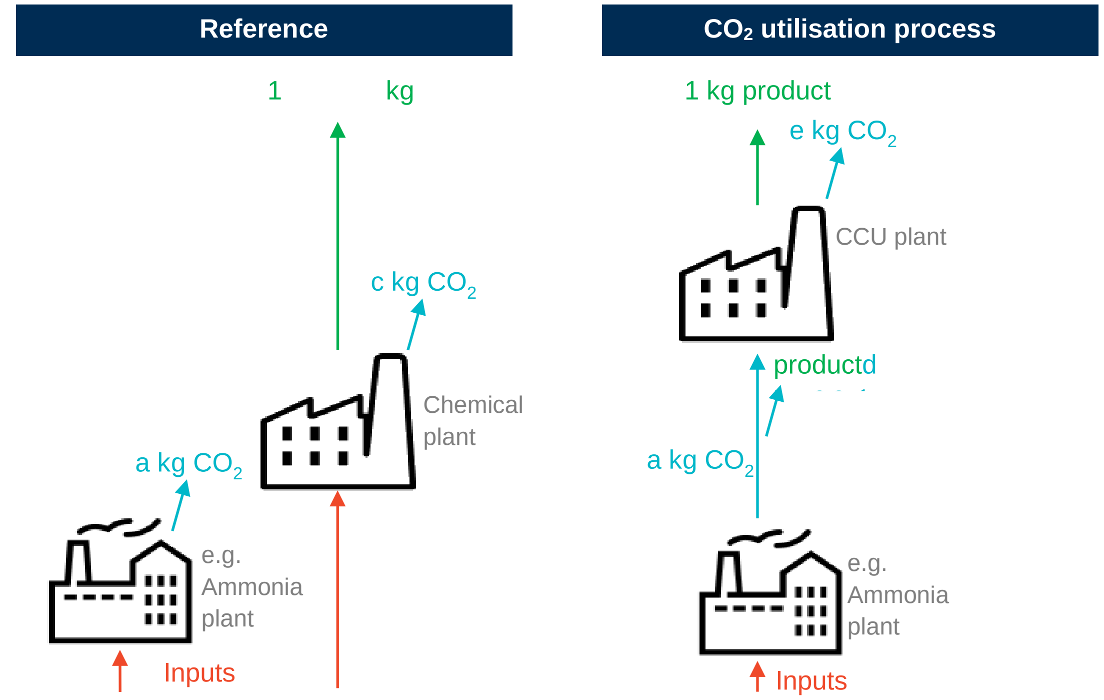
In some cases, pathways simultaneously produce more than one of the products considered in this analysis. This is e.g. the case for the methanol-to-olefin process, which produces ethylene, propylene and toluene. The ratios between those products may vary to some extent. It is not considered as a problem that needs to be treated with a system expansion, but rather consider all products to have the same environmental impact (“1 kg of any olefin produced by this process causes x impact”).

3.4 GHG Credit for CO and CO_2 utilization processes

The investigated processes use CO or CO_2 as a carbon source to replace predominantly fossil carbon in chemicals or fuels. Both are emitted from a process (e.g. steel mills for CO or ammonia production for CO_2). As explained in [1], a full LCA would do a system expansion to include this process in the system boundaries to account for changes in the process or interdependencies. For example, the full functional unit of a steel mill with a CO utilizing process would be 1 kg of product + x kWh of electricity + y kg of steel (because the CO is currently used in an internal power plant to generate electricity). As we are doing a preliminary screening study to compare CO and CO_2 pathways, we wanted to have a functional unit of 1 kg of product where possible. That’s why we decided to use the GHG credit approach explained below.

3.4.1 CO_2 based pathways

One assumption of this study is that CO_2 would otherwise be emitted to the atmosphere. We also assume that the CO_2 utilization doesn’t change the efficiency of the CO_2 producing process. We therefore give the CCU process a credit of 1 kg CO_2-eq/kg used_CO_2. The CO_2 capture and conditioning are accounted for by reducing this credit by the amount of GHG emitted by the capture and conditioning processes. We chose this approach to keep a simple functional unit (1 kg of product).



Balance sheet – CO_2 emissions	Reference	CO_2 utilisation process
Total:	a+c	d[1]+e
Give CO_2 credit to CCU process[2]:	c	d+e-a

Figure 2: Schematic explanation of emitted CO_2 of a CO_2 utilisation process

3.4.2 CO based pathways

CO on the other hand has a high energy content and is already used in most cases to produce heat or electricity. To use the CO in a CO utilisation process, a system expansion is needed. Instead of just capturing the CO, we need to replace its current use. So the real functional unit for the analysis would be 1 kg of product and x kWh of electricity (either produced from CO in the reference case, or produced from the European electricity mix in the CO utilisation case).

For the sake of clarity, we assumed that:

- CO comes from a process that would otherwise use the CO to produce electricity.
- The CCU process gets a credit of 1.57 kg CO_2-eq/kg used_CO because burning one molecule of CO (MW 28) creates one molecule of CO_2 (MW 44). Therefore, by using 1 kg CO chemically rather than burning it avoids the creation of 1.57 (44/28) kg CO_2.
- However, using the CO chemically means that the electricity that would have been generated by burning the CO (roughly 1.5 kWh) now needs to be obtained from the electricity grid. This adds a burden which reduces the 1.57 Kg CO_2-eq credit described above. The burden per kg CO is calculated by multiplying the 1.5 kWh with the CO_2 intensity of electricity from the energy scenarios (see chapter 4.2).

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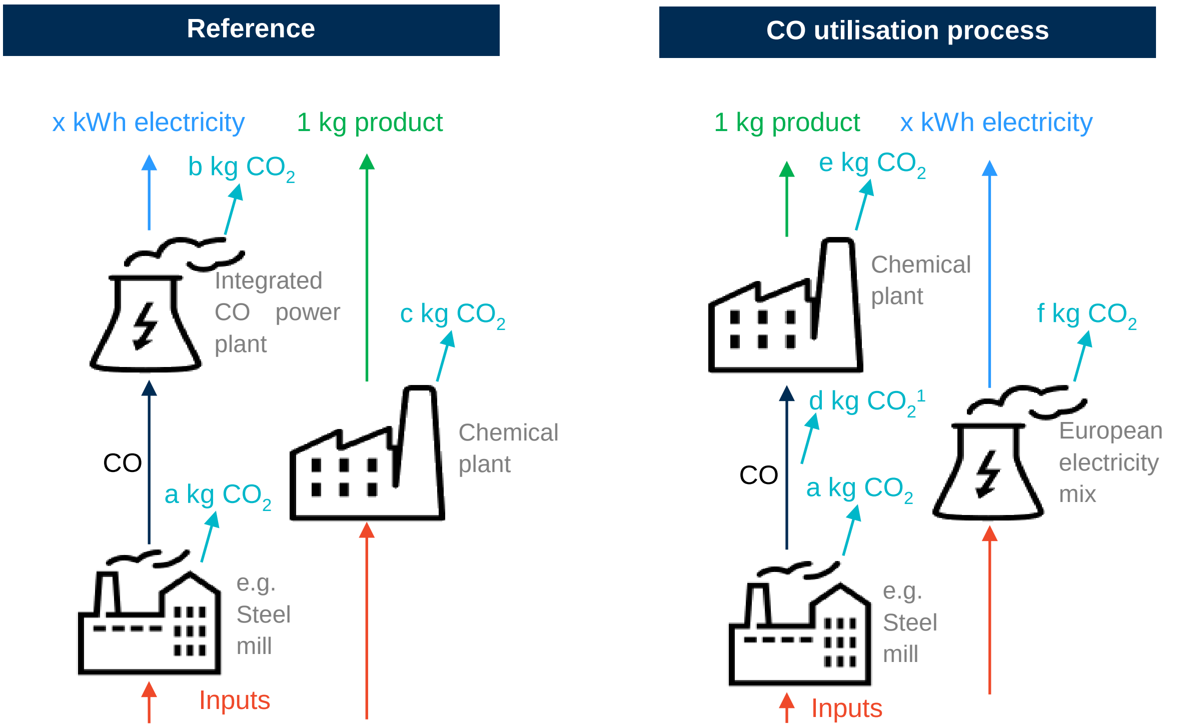
[1] d is the amount of emissions for capture and conditioning of the CO_2 (not needed for the reference).

[2] As we are comparing the CCU and the reference case, we can substract the same value from both sides of the balance sheet.



Balance sheet – CO_2 emissions	**Reference**	**CO utilisation process**
Total:	a+b+c	a+d[3]+e+f
Simplified (no difference in CO supplying process):	b+c	d+e+f
Give CO_2 credit to CO utilization process[4]:	c	d+e+f-b

Figure 3: Schematic explanation of emitted CO_2 of a CO utilisation process

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[3] d is the amount of emissions for capture and conditioning of the CO (not needed for the reference).

[4] As we are comparing the novel and the reference case, we can subtract the same value from both sides of the balance sheet.

4. Methodology for the assessment

4.1 Inventory analysis

Because of the very sparse and disparate data on the selected pathways, we opted for a modular approach. Each pathway will be broken down into processes, and for each process, an inventory analysis will be established, focussing on the main energy inputs (electricity, hydrogen and heat), CO_2 input and greenhouse gas emissions. Those processes will then be assembled in the pathways, paying attention that the temperature and pressure levels of the output of one process correspond to the input level of the next process.

An iterative approach is used as suggested above [4], meaning that in a first step, even approximate data is gathered if no better data is available in order to be able to assess the importance of the different steps, and thus, to refine the results in subsequent iterations.

Electricity, hydrogen, heat and CO_2 are treated as inputs, as their environmental impact can vary strongly depending on the production technology. Four scenarios will be created to cover the breadth of possible environmental impacts of those inputs.

4.1.1 Identifying the technical parameters of the sub-processes

An extensive literature search will be conducted to identify techno-economic analyses and life cycle assessments for process steps included in any of the pathways. The technical parameters like input/output data, efficiency, temperature and pressure levels will be gathered. For some processes, several literature sources were available. In those cases, we checked all sources and either combined them into a “best guess” (in general, using a mean value for diverging in- and outputs) or used the process that seemed more plausible. As chemical processes are highly integrated, the temperature and pressure levels and the heating and cooling needs for each process will be documented to be able to assess integration possibilities with other processes of the pathway. An example of the data collected for a single process is presented diagrammatically in Figure 2below.

Process i	
Pressure:x	Temperature:y
Inputs	Outputs
…	…
…	…

Figure 4: Example of sub-process data

4.1.2 Building the pathways from main inputs to the product

Building on the data for each process step, the pathways will be constructed through simple connection of the inputs of one process to the output of another process, until all inputs are CO_2, CO, electricity, hydrogen and heat (the “main inputs”). This is in line with a general LCA program connecting “unit processes” up to a certain depth and then using cumulative “life cycle inventory” data for the inputs of the remaining inputs. Figure 3 presents this diagrammatically. If the pressure levels between connected processes are different, compression energy will be calculated.

Many of the pathways from CO_2 use syngas as an intermediate product. Four different pathways to produce methanol were chosen that only differ in the syngas production. It was decided that those four routes to produce syngas would be used for all pathways that use syngas as an intermediate.

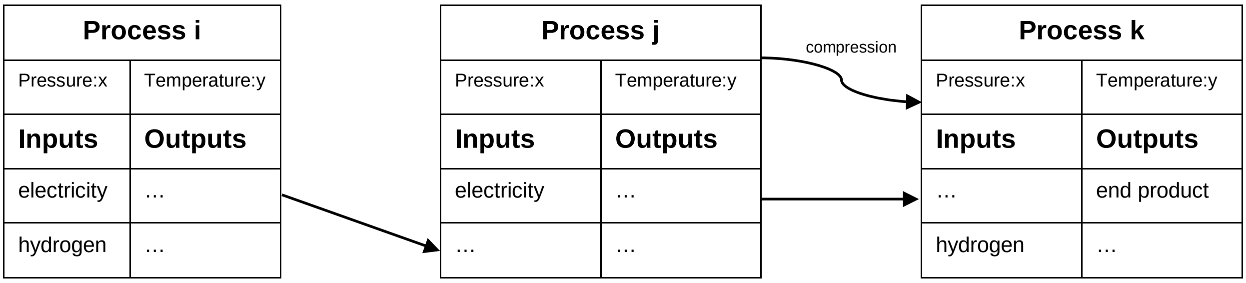

Figure 5: Example of building a pathway from sub-process data

4.1.3 Estimating the plant lifecycle

As data on industrial size plants is almost never available, the whole lifecycle of a plant is considered to be roughly the same as a conventional plant. A particular focus should be put on differences with a high impact, as potentially different catalysts may have. Wherever possible, those catalysts will be mentioned. If LCAs for those catalysts are available, they will be used to identify problematic environmental impacts.

4.1.4 Comparing to current production route

For each product, we will define a reference process. This reference process will be treated in the same way as the CO/CO_2 utilization process, meaning:

- plant lifecycle will only be included if it could be included for the CO/CO_2 utilization process,
- CO_2, CO, electricity, hydrogen and heat will be treated as inputs from the scenarios,
- the system boundaries for the reference processes and the CO/CO_2 utilization process will be cradle-to-gate.

4.2 Scenarios

In line with the methodology from the business cases defined in deliverable 4.1, we will use similar scenarios to allow for the bandwidth of uncertainties and different possibilities regarding the electricity, hydrogen and heat production as well as CO and CO_2 capture. Those scenarios are based on "Guideline for Life cycle assessment of CO_2 Utilization" (a document that will be published this summer) [4], which based them on the IEA 2017 report for meeting the 2 °C target [5] and the GaBi database.

4.2.1 Scenario 1: EU Mix

As a starting point, the current European electricity mix will be used in this scenario. Hydrogen will be produced by steam methane reforming, heat comes from a natural gas boiler and CO and CO_2 capture are based on available technologies, CO_2 being captured from the exhaust gases of a coal-fired power plant and CO from steel mill off-gases.

	EU Mix
GHG emissions electricity [kg CO_2eq/kWh]	0,44
GHG emissions H_2 [kg CO_2eq/kg H_2]	10,70
GHG emissions heat [kg CO_2eq/kWh]	0,26
GHG emissions CO_2 [kg CO_2eq/kg CO_2]	0,15
CO [kg CO_2eq/kg CO]	0,82

4.2.2 Scenario 2: RES ~ 30%

The European electricity mix for 2030 from the IEA report has a significantly lower carbon intensity. On the other hand, CO_2 capture has been switched to direct air capture and therefore causes higher emissions than in the EU Mix scenario. Hydrogen production has been switched to electrolysis.

	RES ~ 30 %
GHG emissions electricity [kg CO_2eq/kWh]	0,15
GHG emissions H_2 [kg CO_2eq/kg H_2]	7,58
GHG emissions heat [kg CO_2eq/kWh]	0,16
GHG emissions CO_2 [kg CO2eq/kg CO_2]	0,23
GHG emissions CO [kg CO_2eq/kg CO]	0,28

4.2.3 Scenario 3: RES ~ 80%

By 2050, electricity production is assumed to be nearly exclusively renewable. Heat is produced by electrode boiler.

	RES ~ 80%
GHG emissions electricity [kg CO_2eq/kWh]	0,06
GHG emissions H_2 [kg CO_2eq/kg H_2]	2,14
GHG emissions heat [kg CO_2eq/kWh]	0,04
GHG emissions CO_2 [kg CO2eq/kg CO_2]	0,06
GHG emissions CO [kg CO_2eq/kg CO]	0,11

4.2.4 Scenario 4: Decarbonized

As hydrogen and heat are produced from electricity and CO and CO_2 capture needs mostly electricity and heat as inputs, all impacts are lowered by switching to a totally “decarbonized” electricity production.

	Decarbonized
GHG emissions electricity [kg CO_2eq/kWh]	0,01
GHG emissions H_2 [kg CO_2eq/kg H_2]	0,67
GHG emissions heat [kg CO_2eq/kWh]	0,01
GHG emissions CO_2 [kg CO2eq/kg CO_2]	0,02
GHG emissions CO [kg CO_2eq/kg CO]	0,02

4.3 Impact assessment

The impact assessment will be limited to the impact “climate change”. Jolliet et al. [6] recommend using the global warming potential GWP100 for the medium term impact and the global temperature change potential GTP100 for the longer term impact of several centuries. As uncertainties are still very high and the main available and recorded data about emissions are from CO_2, we believe that the distinction is not necessary and therefore only present a simplified GWP100. This is done by adding up the GHG emissions arising from electricity, hydrogen, heat, CO_2 and CO from the scenarios and the CO_2 (and where available other relevant emissions like methane) balance from the core process.

4.4 Interpretation

In accordance with the goal of this study, all pathways will be compared with each other and with their respective conventional route. It will be assessed under which circumstances they are energy and carbon efficient. The scenarios will be used to determine effects of different GHG intensities of the main inputs. Figure 4 shows an example of a plot for one pathway over different scenarios. The blue line represents the overall GHG emissions of the CO/CO_2 utilization pathway while the red line represents the reference process GHG emissions. So, whenever the blue line is beneath the red line, the CO/CO_2 utilization pathway is better than the reference. If the blue line is below 0, the pathway is a net consumer of CO_2 (from carbon capture to gate as defined in the scope).

Energy or carbon inefficient pathways that have higher GHG emissions in each scenario than the reference will be excluded.

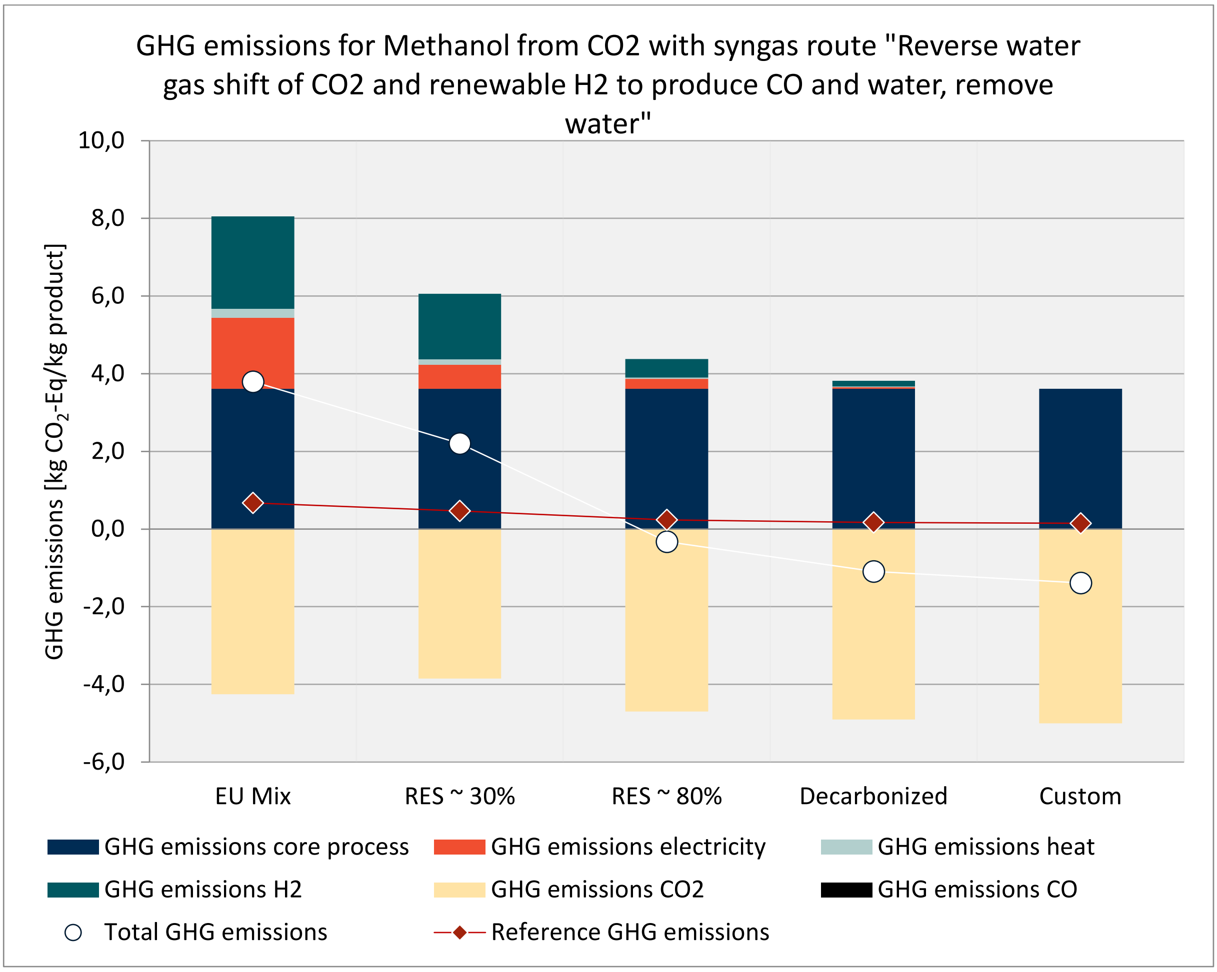

Figure 6: Example of plot showing the influence of the scenario assumptions on GHG emissions

Figure 5 shows a similar plot for one scenario, comparing different pathways. With this analysis, the potentially best pathways for that scenario can be identified. In the example, FT fuels from CO would have the highest GHG savings potential of all displayed pathways within the energy scenario *RES > 30%*.

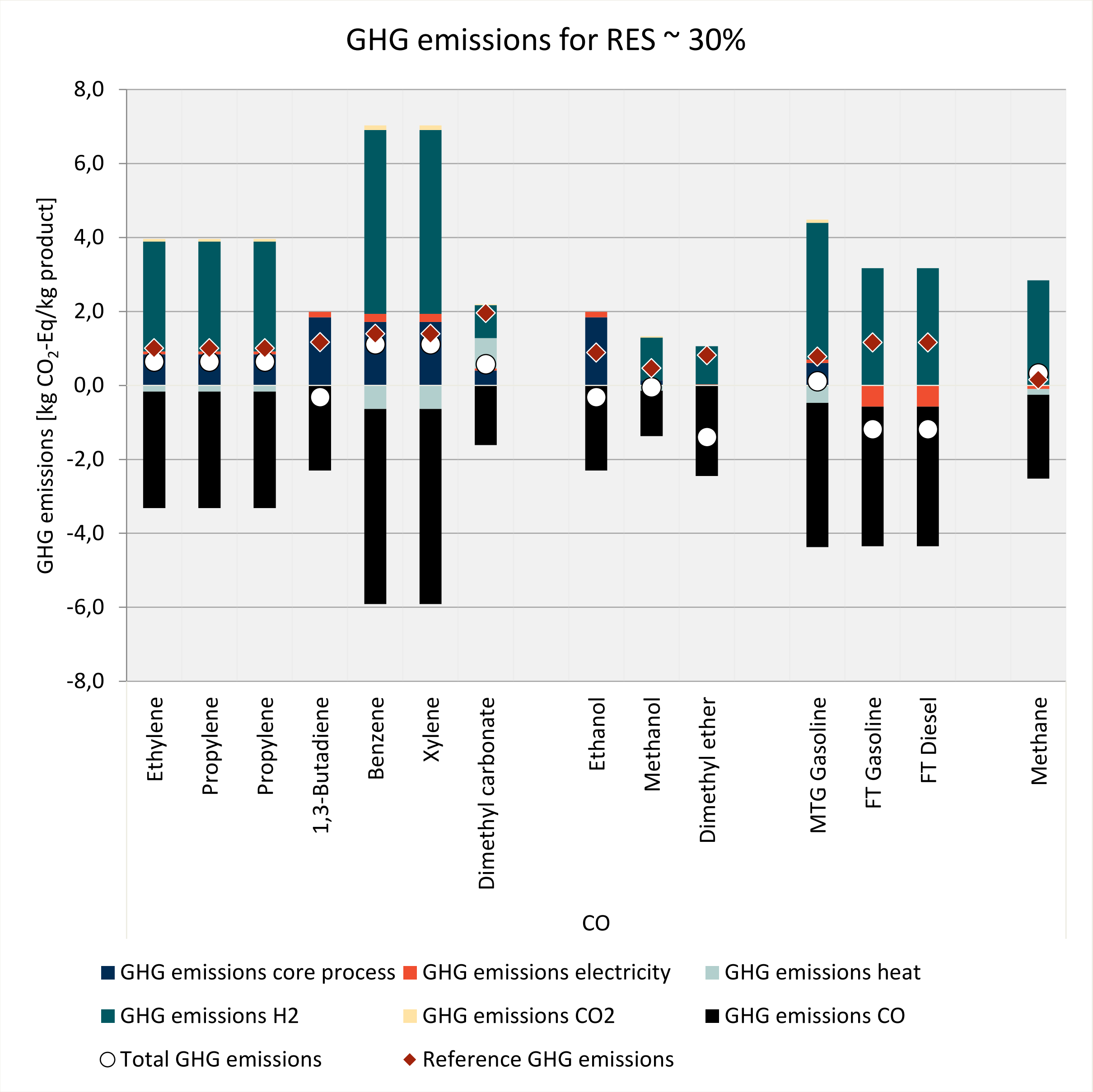

Figure 7: Example of plot showing the GHG emissions of different pathways

4.5 Combination of economic and environmental assessment

Results from the economic analysis and the present environmental analysis will be combined to determine the best overall pathways. If trade-offs are necessary, metrics like GHG mitigation costs or similar will be used. This will be especially interesting for platform chemicals like methanol, where several pathways are analysed. It is important to see if carbon efficient pathways are also economically viable. Figure 6 shows a way to compare pathways with regards to costs and environmental impact via GHG reduction costs. Because of the weak data base and the screening study methodology, the results given by such a highly aggregated metric have to be treated carefully.

In addition, results may vary substantially depending on the energy mix, so this analysis has to be done for each scenario.

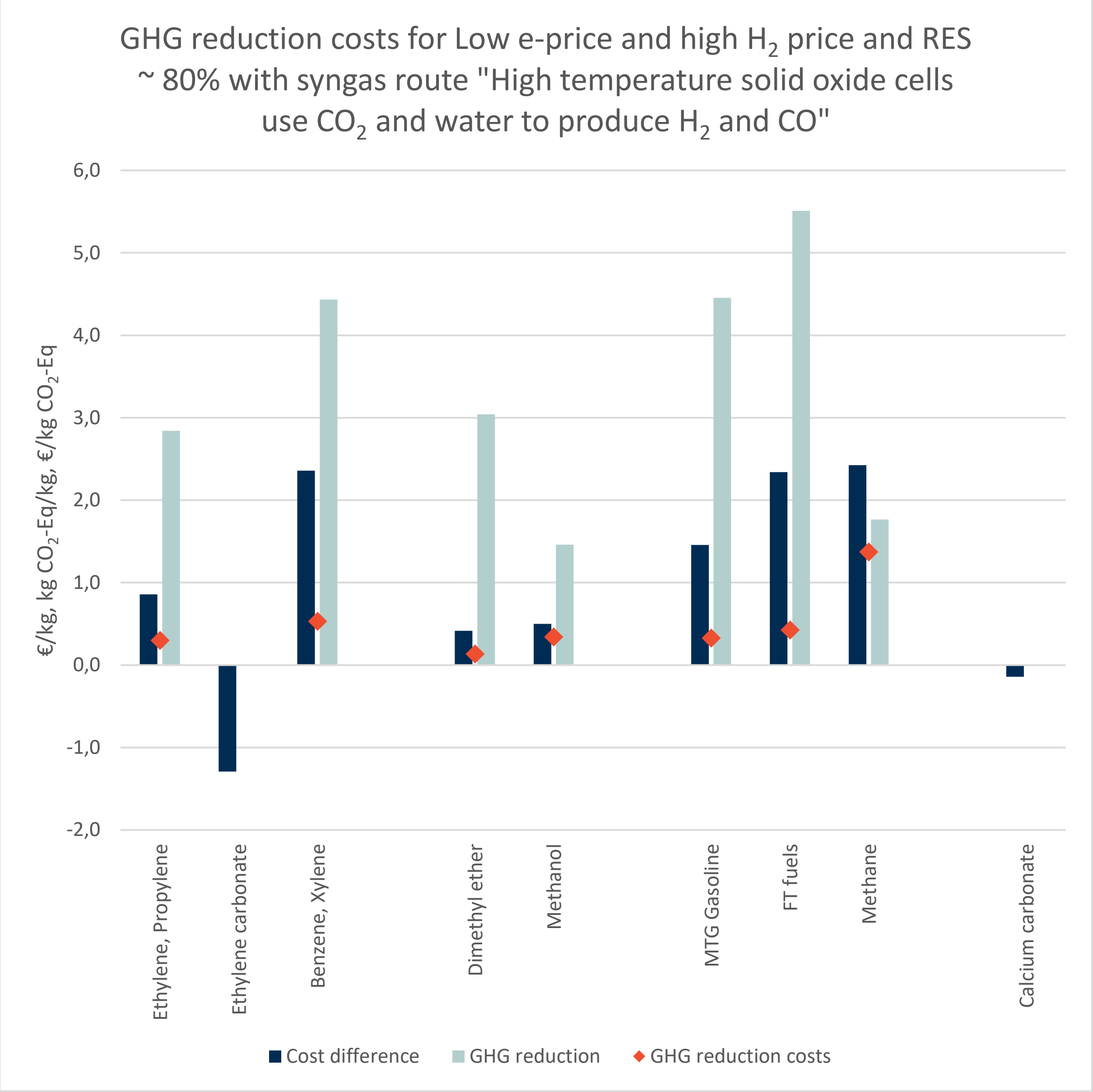

Figure 8: Example of plot showing the GHG reduction costs of different pathways

GHG reduction costs are only available for pathways with net GHG reductions and negative GHG reduction costs don’t have any meaning. They just show that costs are lower than for the conventional technology.

Those pathways with negative GHG reduction costs allow for an easy implementation as the costs and emissions are lower than the reference.

Even if GHG reduction might be high in one pathway, it might be that the market size and structure don’t allow for a large-scale introduction of CCU product. The results are therefore put into perspective by comparing the GHG mitigation and cost difference per kg of product with the market size and also the profit margin where possible. This will allow to see the total potential of each pathway.

5. Bibliography

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