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C2FUEL

Carbon Captured Fuel and Energy Carriers for an Intensified Steel Off-Gases based Electricity Generation in a Smarter Industrial Ecosystem

Deliverable

D6.4 – Goal and scope of the environmental assessment applied to C2FUEL project

WP6 – Technical, economic, and environmental assessment

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Deliverable report

1 Executive Summary

1.1 Description of the deliverable content and purpose

Carbon capture and utilization (CCU) gathers all processes that use CO_2 as a feedstock to convert it into value-added products such as fuels, chemicals or materials. It involves different steps, from capturing the CO_2 from its source to its conversion into carbon-containing products, further including the use of such products up to their disposal as carbon-containing waste. C2FUEL project will develop and test two innovative routes for conversion of CO_2 into chemical energy carriers to be used for mobility applications:

- The first line relates to CO_2 hydrogenation in a membrane reactor with water removal to produce DME. The DME produced will be tested as a fuel for heavy mobility (buses, trucks, boats, etc.) in internal combustion engines.
- The second line relates to the conversion of CO_2 to formic acid through CO_2 hydrogenation or electrocatalytic conversion. Formic acid is one of the most promising hydrogen carriers for massive hydrogen storage and transportation and will be used within C2FUEL in a dedicated genset for electric boats charging at berth.

Besides technical feasibility, economic competitiveness and replication at industrial scale, environmental assessment is crucial as these innovative CO_2 conversion routes and the way the carbon-based products are used must demonstrate reduced environmental impacts against current best available technologies. **As a result, task 6.3 of C2FUEL project is dedicated to the quantification of the life cycle environmental performance of the technological bricks developed in the C2FUEL project.** This assessment will be used to guide the development of the project through key environmental performance indicators and to inform future stakeholders on the performances in order to support their decisions.

Since the goal definition is decisive for all the other phases of the life cycle assessment (LCA), a clear initial goal definition is key for a correct interpretation of the results. It is important to identify what will be studied as well as the depth that will be considered for the modeling and the interpretation. It will be a basis to ensure a common understanding from all partners and interactive dialogue along the project. **This report is split into two sections. The first one presents a state of the art of environmental impacts assessment studies for CO_2 recovery and conversion processes. The second one is dedicated to goal and scope definition of the LCA to be performed within C2FUEL: beyond the goal and scope,**

reference systems for the comparison, data and models to be used for the inventory, environmental impact categories to be included in the assessment.

The task also includes the management of data collection, including data collection templates. This will ensure an efficient flow of information between partners, reducing the risk associated with the data collection process.

1.2 Brief description of the state of the art and the innovation breakthroughs

N/A

1.3 Corrective action (if relevant)

N/A

1.4 IPR issues (if relevant)

N/A

2 Goal and scope of the environmental assessment applied to C2FUEL project

2.1 Introduction

On the one hand, the combustion of conventional fuels within the transportation sector is a crucial driver of global warming and produces a number of harmful emissions. To decrease these adverse factors, the development of synthetic fuels produced from renewable energy sources via the catalytic conversion of carbon dioxide (CO_2) thanks to hydrogen (H_2) has progressed significantly.

One the other hand, the massive development of renewable energy sources involves the probable increase of mismatching occurrence between production and consumption on the electric grid. A solution to avoid these critical issues is to convert renewable electricity into storable hydrogen-based energy carriers.

The C2FUEL project will develop and test two routes for the conversion of CO_2 into energy carriers to be used for mobility applications:

- The first line relates to CO_2 hydrogenation to dimethyl ether (DME) (through methanol or directly) in a membrane reactor with water removal. DME is a promising clean alternative to diesel and the DME produced within the project will be tested into real internal combustion engines.
- The second line relates to the conversion of CO_2 to formic acid (FA) which is one of the most promising hydrogen carriers for massive hydrogen storage and transportation. The formic acid produced within the project will be used in a dedicated genset to produce electricity in Dunkirk Harbour environment for electric boat charging at berth.

This task 6.3 aims at quantifying the life cycle environmental performance of the technological bricks developed in the C2FUEL project. This assessment will be used to guide the development of the project through key environmental performance indicators and to inform future stakeholders on the performances in order to support their decisions.

This study will use the life cycle assessment methodology (LCA), in agreement with the following standards describing its aims and use:

- EN ISO 14040:2006 : Environmental management — Life cycle assessment — Principles and framework

- EN ISO 14044:2006 : environmental management — life cycle assessment — requirements and guidelines

These standards layout requirements and guidelines for: the definition of the goal and scope, the life-cycle inventory analysis phase, the life-cycle impact assessment phase, the interpretation phase and the reporting and critical review of the LCA.

The first step in an LCA is goal and scope definition and the system boundary to clarify what will be studied. It will be a basis to ensure a common understanding from all partners and interactive dialogue along the project. The objective of this document is to present a state of the art on environmental impact assessment studies for CO_2 recovery processes and to present the goal and scope definition for the LCA to be achieved within C2FUEL project.

2.2 Literature review: State of the art on LCA applied to CO_2 recovery processes

Figure 1 presents the most common chemical conversion routes of CO_2 into chemical energy carriers, fuels and fuel additives. Hydrogenation of CO_2 is extensively described in the literature [1] as it provides a direct route to formic acid and methanol, very useful chemicals feedstocks which can directly be used for energetic applications. Other conversion routes such as dry reforming of methane could also be a potential alternative for CO_2 hydrogenation if the produced syngas can be converted into a fuel, preferably methanol or DME, as these are best suited for the replacement of conventional fuels.

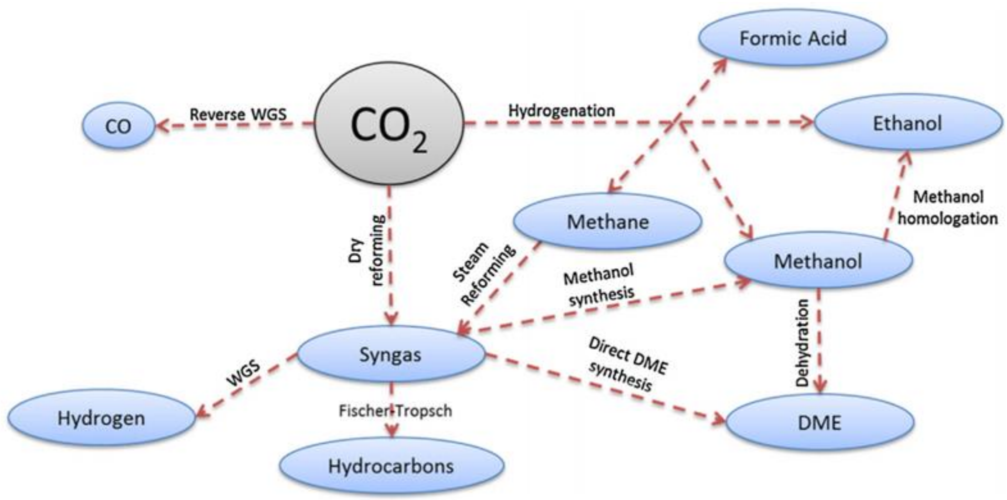


Figure 1: Schematic representation of main production routes of CO2 utilization into fuel [1].

Lots of studies have been conducted for various life cycle assessment of CCU options [2]. Most of them have considered fossil-fuel power plants as a source of CO_2, others have considered the use of CO_2 from chemical plants such as ammonia and hydrogen production plants.

These studies have shown that not all CO_2 sources are equivalent, and the origin of the CO_2 therefore influences the results in terms of environmental performance. The characteristics of the carbon source shall be described within an LCA by the CO_2 concentration, the concentration of other gases and compounds, pressure, temperature and any other specific relevant parameters. CO_2 can also be captured from processes using biomass for anaerobic digestion, fermentation (as production of bioethanol), or gasification. In this case, even if the origin of CO_2 is biogenic, the environmental footprint of the capture shall be taken into account.

For the capture of CO_2, the majority of these studies have considered post-combustion capture with absorption in amine-based solvents [3] such as monoethanolamine (MEA), and the remaining ones have focused on pre-combustion capture including the technology based on the use of selexol [4]. Regarding CO2 capture and conversion through microalgae, all the studies have considered direct injection of flue gases from power plants [5].

As summarized in the Table 3 presented in the Annex 1, specifically regarding FA, the literature review includes two studies to assess environmental impacts using the LCA method for electro-chemical conversion of CO_2 to FA [6,7]. These studies compare LCA of FA production from CO_2 by electrochemical reduction and the production of FA using CO obtained from fossil fuels (conventional method for formic acid production). On DME production from CO_2, one study has been identified in which the methanol and dimethyl ether production from renewable hydrogen and carbon dioxide are assessed [8]. Other LCA studies were identified regarding the conversion of CO_2 into mineral carbonates [9,10, 11], Enhanced Oil Recovery (EOR) [12], and biodiesel from microalgae [13].

2.2.1 Function, functional unit

The functionals units in LCA studies related to CCU (which provides a reference to which the inputs and outputs can be related) are often the production of one kg or ton of chemical product or the production of a given amount of energy. It is important to specify whether the CCU process delivers a product (energy carrier/fuel, chemical, material) or an energy storage service or both, in particular to define the reference system to which it is compared.

2.2.2 System boundaries

According to the guidelines for LCA of CCU supported by the European Commission Directorate-General for Energy (DG Energy) [14], the system boundaries should be "Cradle-to-grave" to assess the environmental impact of a CCU technology. This means that the system boundaries must consider the CO_2 separation and capture from the source, its compression, transport and use options such as chemical synthesis, carbon mineralisation, EOR or biodiesel production (Figure 2). The use phase and end-of-life should be considered too.

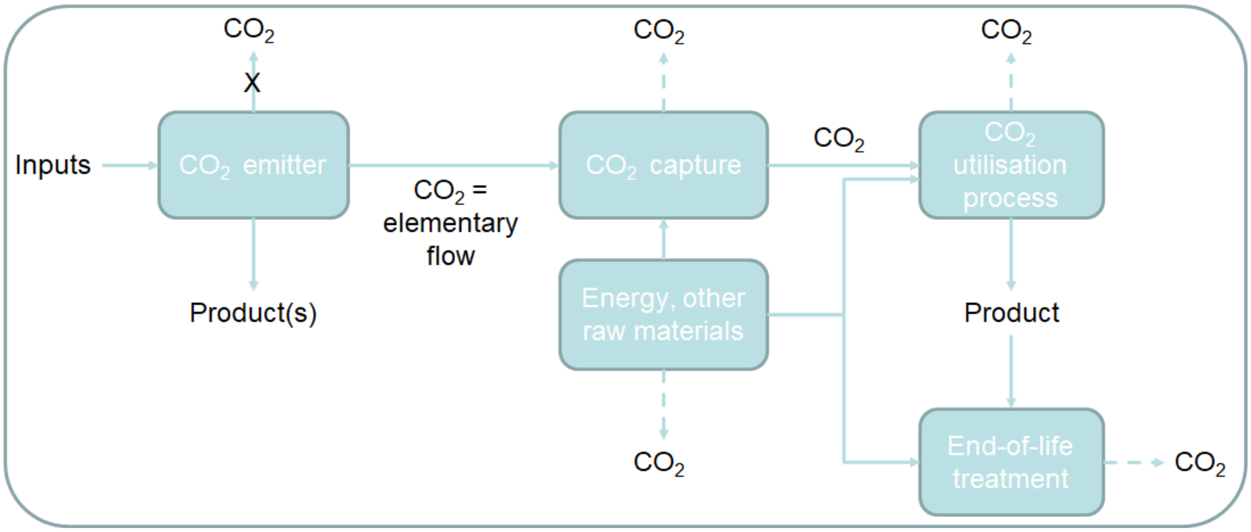


Figure 2: System boundary for CCU: cradle-to-grave

2.2.3 Inventory and data collection

The Life Cycle Inventory (LCI) involves creating an inventory of flows, which include inputs of mass and energy balances, raw materials, and releases to air, land, and water. According to ISO 14040 the data must be related to the functional unit. Related to LCA summarized in the Table 3 (Annex 1), input and output data needed for the construction of the model were collected form: technological bricks at laboratory scale [6], simulations programmes like aspen [8], and completed by available data in the literature and databases like Ecoinvent and Gabi [6,8]

2.2.4 Environmental impact categories

Life cycle impact assessment (LCIA) is used to evaluate the significance of the environmental intervention from the life cycle inventory. Key driver for CCU is to lower GHG emissions and our dependence on fossil resources. Global warming and fossil resource depletion (or fossil-based cumulative energy demand) are usually selected as impact categories in LCA studies on CCU [15]. The

introduction of CCU technologies may further affect a variety of environmental impacts and the holistic LCA approach aims to avoid problem shifting from one impact category to another.
The best practice recommended by the guideline supported by DG Energy [14] is to look at the following full list of impact categories set of CML midpoint impact categories:

- Acidification
- Climate change (biogenic, fossil, Land)
- Ecotoxicity, freshwater (inorganics, metals, organics)
- EF-particulate Matter
- Eutrophication (marine, freshwater, terrestrial)
- Human toxicity, cancer (inorganics, metals, organics)
- Human toxicity, non-cancer (inorganics, metals, organics))
- Ionising radiation, human health
- Land use
- Ozone depletion
- Photochemical ozone formation - human health
- Resource use, fossils
- Resource use, minerals and metals
- Water use

2.2.5 Allocation

Most CCU systems are multi-functional, because CO_2 sources often provide a main product and CO_2 [16]. As discussed above, CCU processes are often compared to conventional processes. To compare both product systems, each product system needs to fulfill the same functional unit and therefore, the system boundaries and the functional unit are changed for the product systems [16].

The DG Energy [14] aims at avoiding allocation wherever possible (and to apply a system expansion approach to include other functions of the product systems). Sometimes however, allocation procedures are required, and as such allocation of CO_2 is one of the most relevant topics in LCA for CCU and also a potential difficulty. In this case the DG Energy [14] recommends to carry out an assessment of the impact of allocation choices as part of the uncertainty analysis.

2.2.6 Uncertainty analysis

Uncertainty analysis remains an indispensable step for LCA of technologies that are not yet commercial [16]. Related to the LCA studies applied to CUU, as most CCU technologies are currently at an early stage of development (e.g., lab-scale) [16]. In the study of LCA applied to the production of dimethyl ether [8] a sensitivity analysis has been conducted on key process parameters in order to explore the operation ranges of the system and to assess the environmental impacts of varying process conditions. Sensitivity analysis also has been applied in the study of formic acid [6] they use approximations, mainly in the energy and infrastructure part. Finally, DG Energy [14] recommended that any LCA of CCU should provide a detailed report of uncertainties (in data, models, allocation choices, etc.).

2.3 LCA applied to C2FUEL project: goal and scope definition

2.3.1 Objectives of the study and targeted public for the results

Within C2FUEL, the goal is to **evaluate the environmental impacts of the new processes developed within the project and to compare them with the conventional routes of FA and DME production.**

The different objectives of the study are to:

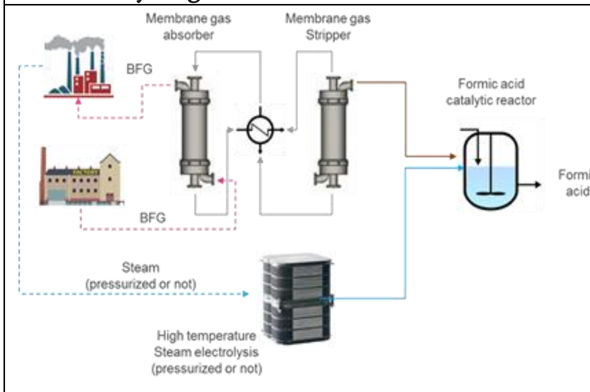
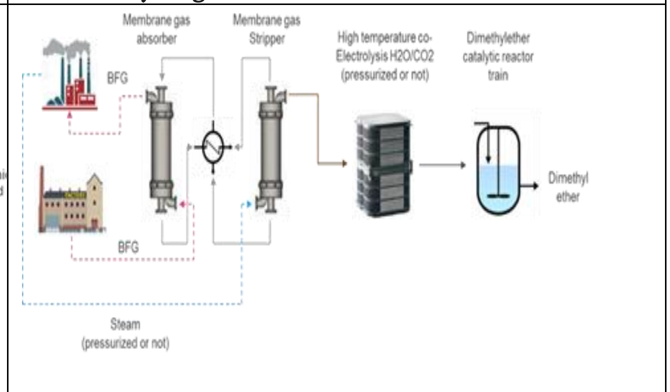
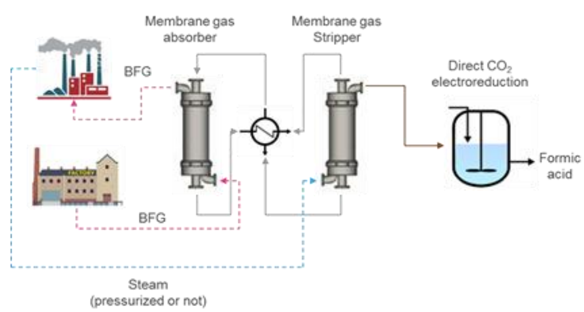
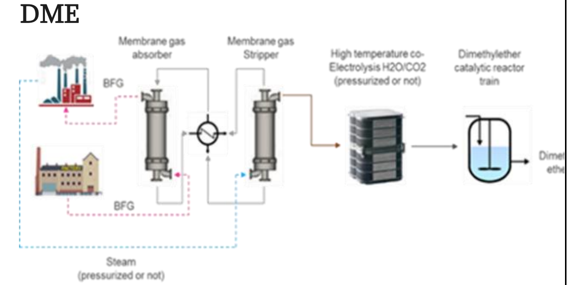
- Conduct a holistic analysis of life cycle environmental impacts of the pathways production and use of formic acid and DME developed in C2FUEL project thanks to LCA methodology;
- Compare the environmental impacts of production and use of formic acid and DME developed in C2FUEL to conventional and innovative production[1] and use. The different possible utilizations of the chemical energy carriers produced are:
    - Formic acid as a hydrogen carrier for hydrogen storage and transportation. A comparison will be achieved with other hydrogen transportation technologies such as liquid hydrogen, ammonia, other hydrogen carriers, etc.
    - DME as a fuel for heavy mobility. A comparison will be achieved with its competitors (diesel, other alternative fuels, etc.).
    - These uses are not exhaustive and other cases may be integrated during the study.
- Identify the main environmental impacts sources in order to consider potential solutions to mitigate them;
- Get scientific robust results to ensure a potential future external communication on the results.

2.3.2 System definition and reference systems for the comparison

Table 1 shows the list of CO_2 recovery pathways that will be integrated into the scope of the LCA study.

[1] DME and FA production pathway developed within C2FUEL can be compared to other innovative production route as the one developed in Fledged project (H2020) for DME (biomass-to-DME).

Table 1: CO2 recovery pathways in C2Fuel project

FA	DME
1- **Hydrogenation of CO_2**	1- **Hydrogenation of CO_2**
	
2- **Electro-conversion of CO_2**	2- **Co-electrolysis for production of syngas then DME**
	

In order to get a meaning out of the results from the LCA of these innovative production pathways, we need to compare them with those obtained from the LCA of conventional production routes:

- The conventional pathway for FA production is the methyl formate route which is currently the most efficient. This production method is described by a standardized process in the ecoinvent database.
- The conventional pathway for DME production is considered to be fossil-based methanol dehydration. The required methanol for this process is assumed to be equal to the average global methanol production as included in the ecoinvent database (reforming of methane) by taking fossil fuels (natural gas) as feedstocks.

2.3.3 System boundaries

The definition of the scope of the study involves the description of the system to be analyzed and its battery of limits and boundaries. This study will take into consideration as recommended by DG Energy: CO_2 separation and capture from the source (Blast Furnace Gas), its compression, and all the technological bricks developed within C2FUEL project: SOEC system for the production of green

hydrogen, CO_2 hydrogenation reactor for the production of formic acid, CO_2 electroreduction reactor for the production of formic acid, CO_2 hydrogenation membrane reactor for the production of DME.
In the processes studied, energy is consumed by all the components showed in the system boundaries considered in our study in Figure 3 and Figure 4. Energy is mainly consumed by steam (/CO_2) (co-)electrolysis to produce hydrogen or syngas. The energy consumed is either coming from waste heat from the power plant or from renewable electricity sources. To avoid allocation as it is recommended by the DG Energy [14], for the comparison of the CCU process with two products (product of CO_2 source and product of CO_2-process) to a conventional system, the main product of the CO_2 source is added to the functional unit and the conventional system is expanded with the CO_2 source without capture (Figures 3 and 4).

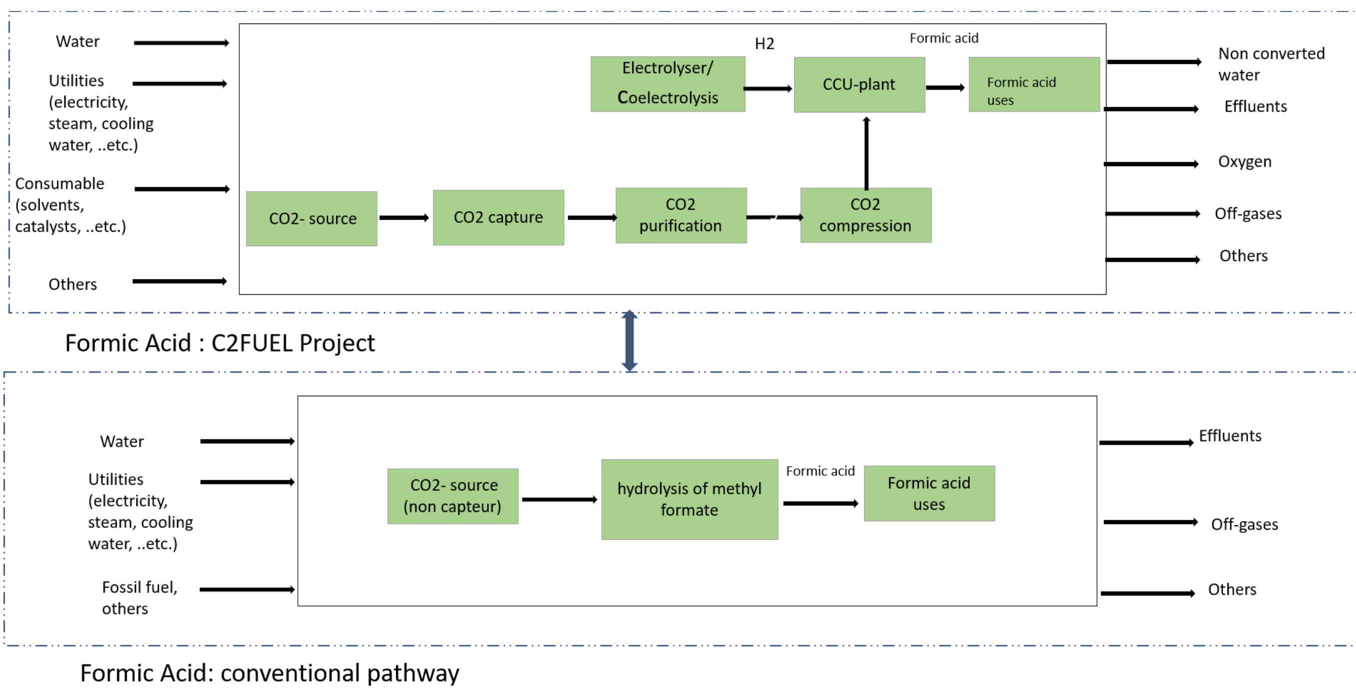


Figure 3: Boundaries of the C2Fuel project towards the boundaries of the most common conventional process for the formic acid production and uses

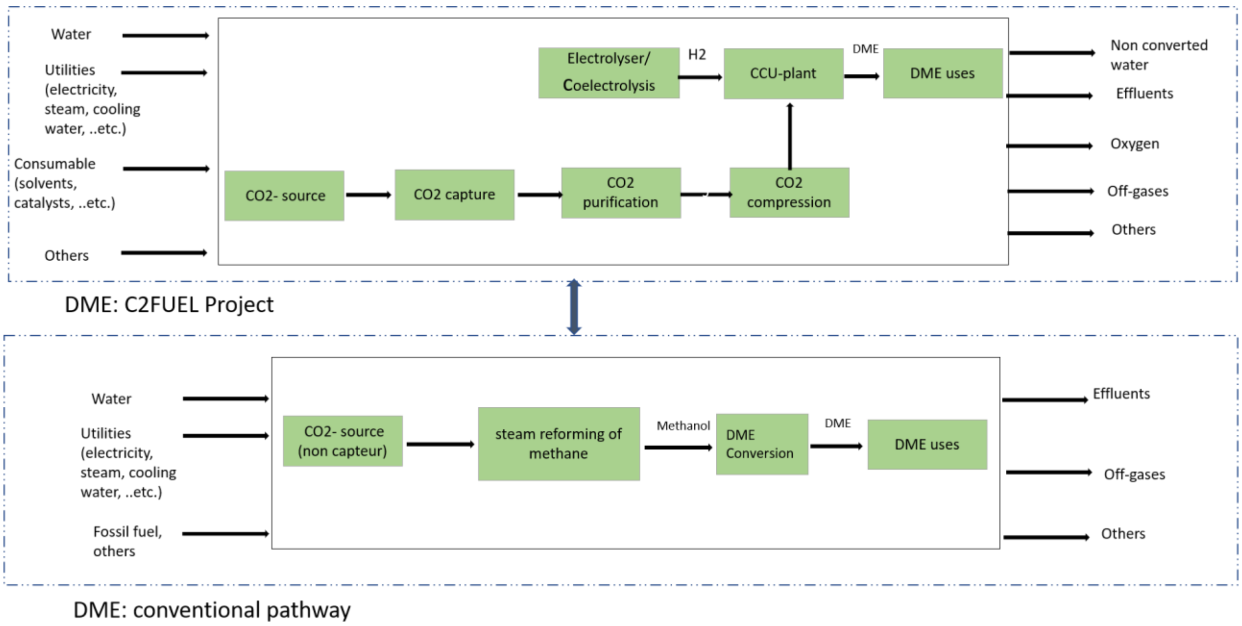


Figure 4: Boundaries of the C2Fuel project towards the boundaries of the most common conventional process for the DME production and uses

2.3.4 Inventory and data collection

The construction of the model must to be collected for all the technological bricks developed in the C2FUEL within the system boundary in collaboration with the projects partners and all along study duration. The data used in this study "which include inputs of mass and energy balances, raw materials, and releases to air, land, and water" will be provided mainly by the project partners, the other data will be provided from the literature and a standard database such as Ecoinvent and Gabi database. Table 2 provides sources and templates of data needed. The management of data collection will ensure an efficient flow of information between partners, reducing the risk associated with the data collection process.

Table 2: Data needed for LCA

Data needed	Data sources	Data collection templates
DME production reactor	TU/e and TECNALIA	Novembre 2020
Formic acid production reactors	TU/e	November 2020
Formic acid reforming reactor and uses	DENS	Novembre 2020
CO2 capturing, conditioning and compressing process	UL/ Ecoinvent database/literature	November 2020
DME uses	BDT and VOLKSWAGEN	Novembre 2020

2.3.5 Life Cycle Impact assessment

In this study, [ENGIE] will evaluate "as much as possible and in function to available data", all of the impact categories, as recommended by DG Energy (see paragraph 2.2.3). A special attention shall be given to GHG emissions and fossil resource depletion (or fossil-based cumulative energy demand) because they are usually selected as impact categories in LCA studies on CCU [15]. The modelling of the LCA will be performed using the Simapro LCA software

By means of an iterative approach, the preliminary LCA results will help identify the most significant contributions to the environmental impacts per indicator and provide recommendations on the most promising configurations and/or scenarios from an environmental point of view, thus guiding eco-design and sustainable integration of the C2FUEL technologies.

2.3.6 Uncertainty analysis and allocation

As the DG Energy [14] recommended that any LCA of CCU should provide a detailed report of uncertainties (in data, models, allocation choices, etc.), a specific work will be conducted within C2FUEL to assess impact of uncertainties on the final LCA results. Regarding allocation aspect, the DG Energy [14] aims at avoiding allocation wherever possible (and to apply a system expansion approach to include other functions of the product systems). If required anyway, following DG Energy recommendation, the impact of allocation choices will be assessed within uncertainty analysis.

2.4 Conclusion

This study is a framework to assess the performance of the C2FUEL technologies. It will be a basis to ensure a common understanding from all partners and interactive dialogue along the project.

This report presented a state of the art on environmental impact assessment studies for CO_2 recovery processes, the goal and scope definition and formulated a first proposal for carrying out for each step of an LCA in the C2FUEL project: goal and scope (functional unit and system boundaries), reference systems, data and models, impact categories.

Next steps are:

- Collect data from the technological bricks developed in the C2FUEL project.
- Perform a preliminary LCA using state-of-the-art based on the relevant ISO. This will identify the most significant contributions to the environmental impacts per indicator and provide recommendations on the most promising configurations and/or scenarios from an environmental point of view, thus guiding sustainable integration of the C2FUEL technologies.

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Annex 1: Summary of LCA studies applied to CCU

Table 3: Summary of some LCA for CCU studies

Study		Scope	Carbon capture method	Utilisation option	Functional unit	LCA impacts
Life Cycle Assessment on the Conversion of CO_2 to Formic Acid	Alvaro Robledo-Diez [6]	Comparative LCA of a CO_2 recovery process by electrochemical route with 2 inputs (CO_2 and H_2O) and 3 outputs (HCOOH, O_2 and H_2 (without addition of chemical materials). And a classic way to produce formic acid from methyl formate (ecoinvent)	CO_2 capture from coal-fired power plant	Formic acid production	production of 100 tons of formic acid 85wt%.	Global Warming Acidification Potential, Photochemical Oxidant Formation, Particulate Matter Formation, Human Toxicity Marine aquatic ecotoxicity potential, land competition and ionising radiation
	Domingues Ramos et al [7]	Comparative 4 LCA to convert CO_2 to formic acid by electrochemic and 2 alternative ways to produce formic acid in ecoinvent	CO_2 capteur is not considered in this study	Formic acid production	production of 1 kg of formic acid 85wt%.	
Production of methanol and dimethyl ether	Michael Matzen [8]	conduct a life-cycle assessment for novel methanol and DME production for use as alternative fuels. wind-based electrolytic hydrogen	CO_2 captured and compressed from an ethanol fermentation process.	methanol and DME production for use as alternative	1 MJ of energy	Global Warming Acidification Potential Photochemical Oxidant Formation Particulate Matter Formation Human Toxicity

Study		Scope	Carbon capture method	Utilisation option	Functional unit	LCA impacts
Mineral carbonation	Khoo et al [9]	LCA of a CCGT plant in Singapore with carbon capture and mineral carbonation (with and without heat recovery), considering mining and shipment of serpentine from two different locations in Australia	Post-combustion capture via MEA	Mineralisation of CO2 into carbonated products used in construction (e.g. as filler material for concrete)	Supply of 1 MWh of electricity from CCGT	Global Warming
	Khoo et al [10]	LCA of a CCGT plant in Singapore with and without carbon capture and two mineral carbonation processes, considering mining and shipment of serpentine from Australia	Post-combustion capture via MEA and direct carbonation of CO2 from flue gas	Mineralisation of CO2 into MgCO3 with applications in construction and land reclamation	Production of 1 MWh of electricity from CCGT	Global Warming
	Nduagu et al[11]	LCA of coal power plant in Canada including coal and serpentine mining and transport, carbon capture, transport and mineralisation	Post-combustion capture via MEA	Mineralisation of CO2 into MgCO3 with potential applications in construction and landfilling	Sequestration of 1 tonne of CO2 in a mineral silicate	Global Warming

Study		Scope	Carbon capture method	Utilisation option	Functional unit	LCA impacts
Enhanced oil recovery (EOR)	P. Jaramillo [12]	LCA of five IGCC plants in the US with carbon capture, compression, transport and use for EOR, including crude oil refining and combustion of refined products	Pre-combustion capture via selexol	Injection into oil field for EOR	Total production of electricity over the projected lifetime	Global Warming
Diesel production from microalgae	Campbell et al. [13]	Comparative LCA of biodiesel production from microalgae in open raceway ponds with canola biodiesel and ultra-low Sulphur diesel in Australia	Direct injection of flue gas from power plant; pure CO2 captured with MEA from ammonia plant	Production of biodiesel	Tonne kilometre (t km)	GWP