



Life Cycle and Technoeconomic Assessment

CCUS Innovation 2.0

Key Knowledge Deliverable 5.3

Key Knowledge Deliverable Cover Sheet

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Description of KKD 5.3 Life Cycle Analysis

This report presents a Life Cycle Analysis (LCA) of the Metal-Organic Framework (MOF) manufacturing system at Promethean Particles and the pilot-scale post-combustion carbon capture system (PC-CCS) at a test site. The LCA was conducted using Simapro and the Ecoinvent database, with separate analyses for MOF manufacturing and its integration into the PC-CCS.

KKDs to be released in full:

D6.4 - Marketing Material Creation

D6.5 - Conference Presentations and Trade-Show Exhibitions

KKDs to be released after redaction:

D3.2 - Control and Safety System Manufacturing

D3.3 - Build of Capture Rig

D4.1 - Installation of Capture Rig

D4.3 - Rig Operation and Decommissioning

D5.1 - CAPEX Technoeconomic Analysis (TEA)

D5.2 - OPEX TEA

D5.3 - Life Cycle Analysis (LCA)

D6.6 - Stakeholder Analysis



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Introduction

The University of Nottingham has conducted a Life Cycle Analysis (LCA) of the Metal-Organic Frameworks (MOFs) production process at Promethean Particles and the operation of a pilot scale MOF-based Carbon Capture plant at a test site in the UK. The methodology and LCA are provided in this report. This study provides the LCA of the pilot scale MOF manufacturing plant and pilot scale post-combustion carbon capture system (PC-CCS) installed at the test site. This is the first study of its kind to model the CapEx of MOF production on the tonne scale, and the first study to model MOF-based carbon capture at pilot scale using real data collected from trials at an operational power station. This LCA is part of project MONET, which is a project funded by DESNZ under the Net Zero Innovation Portfolio (NZIP) CCUS Innovation 2.0 Call 2. This Deliverable report D5.3 (Life Cycle Analysis (LCA)) falls under work package 5 (Life Cycle and Technoeconomic Assessment). The aim of this deliverable is to provide LCA of both MOF manufacture, and its application in a pilot scale carbon capture system, based on real-world operational data obtained during MOF production and construction of the post-combustion carbon capture system. This report audience is Promethean Particles and aims to benchmark the environmental impact of capture carbon using MOFs against competing technologies such as amines.

Life Cycle Analysis Methodology

LCA is based on ISO 14040 methodology [1]. LCA addresses the environmental aspects and potential environmental impacts such as the use of resources and the environmental consequences of releases throughout a product's life cycle from raw material acquisition through production, use, end-of-life treatment, recycling and final disposal. There are four phases in an LCA study, as outlined in Figure 1:

1. the goal and scope definition phase
2. the inventory analysis phase
3. the impact assessment phase
4. the interpretation phase

The scope, including the system boundary and level of detail, of an LCA depends on the subject and the intended use of the study. The depth and the breadth of LCA can differ considerably depending on the goal of a particular LCA. The life cycle inventory analysis phase (LCI phase) is the second phase of LCA. It is an inventory of input/output data with regard to the system being studied. It involves collection of the data necessary to meet the goals of the defined study. The life cycle impact assessment phase (LCIA) is the third phase of the LCA. The purpose of LCIA is to provide additional information to help assess a product system's LCI results so as to better understand their environmental significance. Life cycle interpretation is the final phase of the LCA procedure, in which the results of an LCI or an LCIA, or both, are

In PC-CCS using MOFs, flue gas with a partial pressure of 0.13-0.16 bar at 40-60 °C is flowed over a MOF-based packed-bed reactor system [28]. The CO₂ adhere to the MOF surface via Van der Waals interactions or covalent bond formation. After saturation, the CO₂ is regenerated via a temperature (up to 200 °C) or pressure swing from the MOFs [29]. Numerous MOFs have been analysed for PC-CCS applications [22, 30]. MOF Mg-MOF-74 possesses the highest working capacity for PC-CCS at 5.87 mmol g⁻¹ at ambient temperature [28]. However, MOF UTSA-16 exhibits higher selectivity for CO₂ over N₂ [31].

Most post-combustion carbon capture LCA studies have been conducted on chemical adsorption using MEA [32]. Most LCA studies of MOF and PC-CCS assess the performance of MOF based on their properties or on the performance of the separation step alone [33-36], and thus an entire life cycle of the process needs to be considered. LCAs of MOFs have found that the use of solvents in MOF production plays a crucial role in their sustainability, and greener alternatives such as methanol and water should be considered along with improved recycling rates [37]. To date, there are no reported comparisons of MOF and amine scrubbing PC-CCS LCA studies. Martin and Flanagan [38] recently compared amine and ammonia based PC-CCS in coal fired plants using Simapro software.

Project MONET: Goal and Scope

The goal of this LCA is to assess the environmental impact of capturing carbon dioxide (CO₂) from the flue gas at the test site using a pilot scale PC-CCS using a MOF as the sorbent. Its scope includes raw materials, manufacturing, and the carbon capture process (use phase) of the MOF. End of life is not included in the analysis. It does not include any downstream systems such as Carbon storage and transport, or any upstream processes where the flue gas originates from. The functional unit was determined to be one hour of carbon capture operation using pressure-vacuum swing adsorption (PVSA) and a defined mass of MOF. Greenhouse gas (GHG) emissions were the primary concern of this analysis; therefore Global Warming Potential (GWP) (kg CO₂ eq) was chosen as the main impact category to be analysed. The impact assessment was performed midpoint, using “ReCiPe 2016 Midpoint (H) V1.08 / World (2010) H” methodology. SimaPro 9.6.0.1 was used for the analysis with the Ecoinvent v3.10.

Project MONET: Life Cycle Inventory

A life cycle assessment model was developed based on the manufacturing process of MOF and the PVSA test rig used by Promethean Particles in the project. The process model used in the analysis is shown in Figure 2, where the life cycle inventory (LCI) data was obtained either from Ecoinvent 3.10 or USLCI (U.S. Life Cycle Inventory) databases. The study is limited by the fact it is based on the pilot-scale data not full-scale manufacturing data. Thus, the data

used is based on pilot-scale production, not an optimised full-scale production of MOF. Furthermore, Promethean Particles are MOF manufacturers, not developers or providers of carbon capture system. Whilst a demonstrator plant has been produced as part of this project, this is not the primary business objective of Promethean Particles, and thus the costs for future carbon capture systems would vary based on the design of the system. Whilst this is one of the largest MOF PC-CCS demonstrators to date, it is not full scale, and thus future LCA will be required for the full-scale production of MOF and capture of carbon dioxide for a true comparison with other full scale carbon capture technologies.

The LCA was developed in Simapro with parametrisation, making it easy to changes values or assumptions in the model. In SimaPro, parameters can be defined on database, project or process level. The parameter list is provided in Table 1.

Table 1 – List of Parameters in the Simapro Model

Parameter	Description
mfg	Flue gas mass flow rate (kg/h)
CO2_In	% of CO2 in Flue gas
H2O_In	% of H2O in Flue gas
O2_In	% of O2 in Flue gas
N2_In	% of N2 in Flue gas
Ar_In	% of Ar in Flue gas
CO2_C	% of CO2 captured (relative to total flue gas "mfg")
H2O_C	% of H2O captured (relative to total flue gas "mfg")
O2_C	% of O2 captured (relative to total flue gas "mfg")
N2_C	% of N2 captured (relative to total flue gas "mfg")

Ar_C	% of Ar captured (relative to total flue gas "mfg")
CO2_Out	% of CO2 in clean gas (relative to total flue gas "mfg")
H2O_Out	% of H2O in clean gas (relative to total flue gas "mfg")
O2_Out	% of O2 in clean gas (relative to total flue gas "mfg")
N2_Out	% of N2 in clean gas (relative to total flue gas "mfg")
Ar_Out	% of Ar in clean gas (relative to total flue gas "mfg")
W_MOF	Total weight of the MOF used in the PVSA system
MOF_CT	MOF cycle time (hour)
MOF_NC	Total number of cycles during MOF lifetime
TD	Transportation distance (lorry, km)
Rsw	Reactor process solvent waste (%)
Piw	Shaping inert waste (%)
Er	Reactor electricity consumption (kWh)
Ew	Washing electricity consumption (kWh)
Ec	Processing electricity consumption (kWh)

Eo	Oven electricity consumption (kWh)
Ep	Shaping electricity consumption (kWh)
Ws1	Weight of solution 1 (kg)
Ws2	Weight of solution 2 (kg)
Wdry	Weight of the intermediate dry MOF
Wwet	Weight of the intermediate wet MOF
Ww	Weight of the intermediate
Wman	Total weight of the dry MOF
Dprc	Distance parameter 1
Dcp	Distance parameter 2
Dppr	Distance parameter 3
Dprd	Distance parameter 4
Eib	Inlet blower electricity consumption (kWh)
Eac	Air cooler consumption (kWh)
Eth1	Tank heater 1 consumption (kWh)
Eth2	Tank heater 2 consumption (kWh)
Evp	Vacuum pump consumption (kWh)
Wsw	Process waste 1 (kg)

Csw	Process waste 2 (kg)
MOF_Life	Lifetime of MOF (hours)
W_MOFFU	Life Weight of MOF per one functional unit (kg/h)

All transportation weights, distances, and the energy consumption of all the manufacturing processes (except transportation) can be individually adjusted.

MOF Manufacturing Life Cycle Analysis

The Life cycle inventory, including SimaPro process names, parameters and Ecoinvent and USLCI database processes for the MOF Manufacturing LCA was collated but is not shown in this report to maintain confidentiality over Promethean’s manufacturing processes.

Recommendations have been provided to Promethean Particles on routes to improve the cost efficiency of the MOF manufacturing process, and significantly reduce the carbon emissions, particularly as production volumes increase.

Carbon Capture Life Cycle Analysis

The PC-CCS LCA includes the manufacturing for a defined volume of MOF. Table 2 provides the Life cycle inventory, including SimaPro process names, parameters and Ecoinvent and USLCI database processes for the PC-CCS system. The quantities used varies by scenario.

Table 2 - Life cycle inventory, including SimaPro process names, parameters and Ecoinvent and USLCI database processes for the PC-CCS System

SimaPro process	Material or Energy [SimaPro parameter]	Database process name
Inlet blower	Electricity [Eib]	Electricity, biomass, at power plant/US System
Air cooler	Electricity [Eac]	Electricity, biomass, at power plant/US System
	Wastewater	Wastewater, average {Europe without

	(see Table 1)	Switzerland} market for wastewater, average Cut-off, S
Tank heater 1	Electricity [Eth1]	Electricity, biomass, at power plant/US System
Tank heater 2	Electricity [Eth2]	Electricity, biomass, at power plant/US System
Vacuum pump	Electricity [Evp]	Electricity, biomass, at power plant/US System
CO2 capture (PVSA,MOF) (h)	Captured gas	n/a
	Flue gas [mfg]	n/a

Project MONET: Functional Unit

Currently most LCA studies on PC-CCS use an electricity based functional unit such as kWh [9]. These studies tend to analyse the whole plant including power generation [10-12]. However, the functional unit for comparing carbon capture systems should be 1 ton of captured CO2 not a unit of energy (1 kWh) as the main purpose of the study is to compare the environmental benefits of CO2 separation systems [9]. This provides a more direct comparison based on the CO2 uptake efficiency. By selecting other functional units, CO2 capture will often appear to be a secondary function of the study, which can make decarbonisation appear less attractive [13]. The selection of the system boundary, functional unit and allocation method are the most relevant methodological choices in PC-CCS studies [14]. Furthermore, comparative studies should exclude processes that are common to two scenarios in order to focus the study on the environmental benefits of the PC-CCS systems of interest [15]. A CO2 based functional unit has been used to compare PC-CCSs using potassium carbonate and monoethanolamine solvents [16], membrane separation and amine scrubbing system [17], and CO2 mineralization [18]. Thoneman and Pizzol [19] also used 1 kg of CO2 as the functional unit to compare 12 different CO2 conversion technologies in the chemical industry. The amount of MOF per functional unit (one hour of operation) is dependent on the MOF cycle time and number of cycles per MOF lifetime and calculated using parameters as follows:

$$\text{MOF_Life} = \text{MOF_CT} \cdot \text{MOF_NC (h)}$$

Where:

MOF_Life : MOF lifetime (h)

MOF_CT : Cycle time (h)

MOF_NC : Number of MOF cycles per lifetime

From here the amount of MOF for one hour of operation:

$$W_{\text{MOFFU}} = \frac{W_{\text{MOF}}}{\text{MOF}_{\text{Life}}} \left(\frac{\text{kg}}{\text{h}} \right)$$

Where:

W_{MOFFU} : Weight of MOF per one functional unit (kg/h)

W_{MOF} : Weight of the MOF installed in the system (kg)

MOF_{Life} : MOF lifetime (h)

Project MONET: Flue Gas Composition

During the PVSA carbon capture process the flue gas is designed to be taken into the system by the inlet blower after which it passes through a pre-treatment system. For LCA modelling, the amount of wastewater leaving the system was approximated to be equal to the water content of the flue gas itself, and is controlled by parameters of the flue gas. This is based on data recorded during project PICASSO, which was funded by a UK Carbon Capture and Storage Research Centre (UKCCSRC) Flexible Fund grant in 2021, and was a precursory project to MONET. In project PICASSO, a proof-of-concept, lower TRL pilot MOF carbon capture rig was installed in a test site. The flue gas composition in project MONET was only measured on the outlet for CO₂. The design case model was based on the flue gas data from project PICASSO as the flue gas information was not available at that time, whilst the pilot scale model is based on the flue gas composition from the MONET trials.

The flue gas is assumed to be dry for the LCA model as it passes through the two MOF columns, operating in parallel, where most of its CO₂ content is captured and is subsequently desorbed by a vacuum pump at the end of each cycle. The pilot PC-CCS is designed to heat the columns intermittently when the MOFs have adsorbed too much residual water in the flue gas stream, and require thermal treatment as a “super regeneration” step to dry the MOF and reinstate its working adsorption capacity. The “super regeneration” was not included in the LCA model as the model assumes the flue gas is dry when it enters the columns. The energy consumption of the test rig was based on energy meter readings from the pilot scale system and was modelled as electricity produced from biomass (excluding losses and transportation) based on U.S. (USLCI) data. The clean gas leaving the system is assumed to be released to the atmosphere and is the difference between the input flue gas and the captured gas. Since the captured gas is modelled as having a negative impact, the emissions from clean gas comes from the “uncaptured” share of the flue gas, and is therefore accounted for in the carbon capture process as modelled in SimaPro “CO₂ capture (PVSA,MOF) w flue gas (per hour)”.

PC-CCS LCA Modelling Uncertainties

There are several uncertainties in the model:

- The number of cycles during MOF lifetime is based on theoretical calculations
- Electricity for the PVSA process is modelled using a plant available in the USLCI database. This process excludes transportation and losses from transmission (electricity available at the power plant). The GWP emissions (kg CO₂ eq) of the USLCI electricity are 15% of the GB mix using Ecoinvent 3.9.1. It is important to note that the emissions at the test site may be different to those included in the model.

Carbon Capture Rig Modelled Scenarios

The original intention of this model was to use pilot scale data from the PC-CCS rig installed at the test site and analyse the different testing configurations. However, due to challenges encountered, the approach was restructured and this test data represents the best adsorption data available. Mitigation steps ultimately meant that the design capture capacity of the system was not demonstratable using the current set up. There were also difficulties in effective capture of the carbon dioxide by the MOF due to water presence in the flue gas when entering the adsorber column, due to ineffective dehydration by the pre-treatment system. Other CO₂ adsorption systems commonly have molecular sieve units installed to dehydrate the gas prior to CO₂ capture and thus this would need to be retrofitted and tested to verify that dehydration of the flue gas overcomes the challenges encountered. Due to the absence of trial data for the operating energy data associated with dehydration, this pre-treatment step has not been included in this model. The test data available has been extrapolated for annual usage and two test scenarios are provided. The original design case which uses the design capture rate, and the pilot scale data.

Scenario 1: Original Design

The LCA model was developed in February 2024 based on the original design data. The capture efficiency is based on the results from project PICASSO, which was 89%. During the model development, the power data was provided by the EPC for the electricity rating of the PC-CCS rig. In addition to energy, there was wastewater from the air cooler, which represents the water removal from the flue gas. The manufacture of the components used in the PC-CCS were not included, and thus only the use phase of the life cycle was considered in this model. The model includes a defined volume of the MOF, and its manufacture is incorporated into the model.

Whilst the vast majority of the GWP impact is associated with the flue gas and captured carbon dioxide, the other impacts are related to the other parts of the PC-CCS. The PC-CCS is the dominant contributor to several categories including stratospheric ozone depletion, ozone formation, and fine particulate emissions. These emissions are related to the electricity

production, potentially due to refrigerant use within the systems, but this was not clear from the Ecoinvent database analysis of this process.

Scenario 2: Pilot Scale Data

Scenario 2 assumes that under cyclic conditions each column would operate in adsorption mode up to a breakthrough threshold. This amount of CO₂ would then be desorbed while the other column enters adsorption mode. The pilot data for the quantity of CO₂ adsorbed until breakthrough is exceeded and the desorption time to desorb this quantity is used to calculate the adsorption capacity, adsorption cycle time, desorption cycle time, and extrapolate to the total capture per annum. The information was generated using the Pilot Scale Data Model in Simapro.

The energy data from the PC-CCS rig was recorded using an Elcomponent Energy Pro energy meter, with data being processed in the PowerView PV2.221 software supplied with the energy meter. The energy meter is installed at the distribution board, and thus reads the electricity draw of the whole rig.

Based on the pilot data, the carbon capture efficiency has dropped significantly compared to scenario 1: design case, which was largely due to a decrease in incoming flow rate of gas, ultimately as a result of the flue gas temperature being significantly lower than anticipated. The available carbon dioxide in the flue gas has reduced from the design case. There is a lower concentration of CO₂ in the flue gas and the volumetric flow rate of the system has been reduced. This is a limiting factor on the operation of the system given it was designed for higher flowrates.

As with scenario 1, the vast majority of the GWP impact is associated with the flue gas and captured carbon dioxide, whilst the other impacts are related to the other parts of the PC-CCS. The PC-CCS is the dominant contributor to several categories including stratospheric ozone depletion, ozone formation, and fine particulate emissions.

Comparison of Scenarios 1 & 2

The potential carbon dioxide available for capture is significantly different between the two scenarios. Due to the equipment originally being designed for the design case, the electricity consumption of both scenarios is the same. This, combined with the lower capture efficiency of the pilot scale case means that the total carbon emissions are very similar for both cases. Thus, neither option are carbon neutral or carbon negative. The results show that the current pilot scale configuration will require significant improvement if it is to achieve its original target. Due to limitations in the design of the PC-CCS, and in data acquisition, it is not possible to state what improvements would be required at this time.

Conclusions

This report provides a summary of the Life Cycle Analysis (LCA) of the MOF manufacturing system at Promethean Particles and the pilot scale post-combustion carbon capture system (PC-CCS) installed at the test site. The LCA was done in Simapro using the Ecoinvent database. The LCA of the MOF manufacture was analysed separately and as part of the PC-CCS. Manufacturing data from Promethean Particles' manufacturing facility in Nottingham was used for the MOF manufacturing LCA, and the PC-CCS LCA was based on pilot scale data where possible.

The results from the MOF manufacturing LCA identified routes for further reduction in carbon dioxide emissions and Global Warming Potential (GWP), and recommendations have been made to Promethean Particles.

Due to limitations in data collection from the pilot scale rig, two scenarios were modelled for the PC-CCS. The first is the original design case and the second model used pilot scale data. This was partly due to the reduced flue gas supply to the rig, but also due to the competitive adsorption of water which caused regeneration challenges for the MOF. Both of these challenges arose as a result of the incoming flue gas temperature being significantly lower than anticipated, or that the pilot PC-CCS was designed for, but also limitations in the current pilot PC-CCS design. Other CO₂ adsorption systems commonly have molecular sieve units installed to dehydrate the gas prior to CO₂ capture and thus this would need to be retrofitted and tested to verify that dehydration of the flue gas enables MOF regeneration. Due to the absence of trial data on operating energy associated with dehydration, this aspect has not been included in this model.

The majority of the GWP of the PC-CCS is associated with the carbon not captured by the system, and the energy used to operate the system. The PC-CCS is the dominant contributor to several categories including stratospheric ozone depletion, ozone formation, and fine particulate emissions. Due to the limited data from the pilot PC-CCS, it is difficult to pinpoint key carbon reduction strategies, especially given the reduction in the operation flue gas flow rate and the future requirement for water removal in system, both of which would have significant impacts on energy. However, it is clear that the higher the capture efficiency of the MOF-based PC-CCS, the lower the overall GWP impact will be as less carbon dioxide will be released to the atmosphere.

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