Promethean Particles®

Life Cycle and Technoeconomic Assessment

CCUS Innovation 2.0

Key Knowledge Deliverable 5.2

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Key Knowledge Deliverable Cover Sheet

This Key Knowledge Deliverable (KKD) has been produced by the University of Nottingham as part of the Department for Energy Security and Net Zero £1bn Net Zero Innovation Portfolio (NZIP) - CCUS Innovation 2.0 programme. The document is reflective of the status of the project at the time of writing. The material presented could have been subject to change as the project matured. These documents should not be considered a full representation of the final project.

Description of KKD 5.2 OPEX TEA

This report presents a techno-economic assessment (TEA) of a carbon capture pilot plant installed at a test site CCUS (Carbon Capture, Utilisation and Storage) Incubation Area. The system employs a metal-organic framework (MOF) to capture CO_2, with updated capital (CAPEX) and operational (OPEX) expenditure estimates for both MOF production and the carbon capture process presented here.

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

Contents

Process Description

The pilot scale MOF-based CO2 capture system consists of two adsorber vessels loaded with shaped MOF produced by Promethean Particles, and is installed at the test site. The scope of this TEA covers the unit operations in the capture system, and no consideration is given for CO2 storage and transportation at this stage as the focus of the pilot trials is on MOF performance. All equipment in the system is costed and the associated operating costs (i.e., electricity use and wastewater treatment) have been costed. The MOF loaded into the vessels has been costed based on data provided by Promethean Particles and is outlined later in this report.

Data Use and Quality

The mass and energy balance and cost data used to create the TEA is based on data from trials of the MOF-based CO2 capture system installed at the test site. Table 1 details the data and assumptions used in the study.

An uncertainty rating for each assumption in the model has been allocated by assessing the quality of the data source and the impact of the assumption on the model outputs. Table 2 provides the definitions for the quality and impact ratings used, and Table 3 shows how these translate into uncertainty ratings for the assumptions made.

Table 1 – Performance and cost data sources used in the TEA

Data	Source
Performance	
Capture rate (kg/yr)	CO2 removal from pilot trials
Electricity usage (kWh/cycle)	Electricity meter data from trials
MOF loading (kg/adsorber)	Amount loaded for trials
Cycle time (minutes/cycle)	Adsorption and desorption time from pilot trials
Waste water generation (m3/cycle)	Measured flue gas water content

Cost	
Capital cost for MOF production plant (pilot scale)	Provided by Promethean
Variable operating cost for MOF	Provided by Promethean
Labour time for MOF production	Provided by Promethean, used to account for labour costs in production
Capital cost for CO2 capture rig	Provided by Promethean

Table 2 – Quality and Impact Rating Definitions

Rating	Definition	Grade	Explanation
Quality Rating	This assesses the certainty and/or robustness of a data source. If the data is manipulated or transformed in some way, the quality decreases. A wide confidence interval (eg ±50%) would have a low quality rating.	High	The value is based on real data and transformations are minimal or robust. The data is current and there is a narrow confidence interval.
		Medium	Value is based on limited data, but reasoning is robust. There has been significant manipulation to the data and the confidence interval is wide.
		Low	There is either no data source or an unreliable data source has been used. Quality rating may also be low if a robust data source is used but the data is likely to change significantly over the model period.
Impact Rating	This assesses the sensitivity of the model outputs to variations in inputs. Rating should reflect the relative change in output when input value is changed.	Low	A change in input value has negligible impact on model outputs.
		Medium	A change in input value has some impact on model outputs.

		High	A change in input value has significant impact on model outputs and could affect decision making.
Uncertainty Rating	This assesses which assumptions need to be highlighted.	Low	Assumption has low impact and source is of good quality. Very little can be done to improve.
		Medium	Assumption has medium impact on model outputs. Changes would affect results but not significantly.
		High	Assumption has high impact on model outputs. Changes have the potential to affect results significantly.
		Very High	Assumption has a very high impact on model outputs. Changes are likely to affect results significantly.

Table 3 – Summary of uncertainty ratings based on impact and quality rating

Uncertainty Rating		Impact Rating		
		Low	Medium	High
Quality Rating	High	Low	Medium	High
	Medium	Low	High	Very High
	Low	Medium	Very high	Very High

MOF Production Cost

As the Continuous Flow Synthesis (CFS) plant manufactures a novel (non-commercial) MOF the production cost is calculated based on the process conducted by Promethean Particles.

The production cost was calculated based on defined production campaign volumes, and scaled to a defined unit volume for use in the TEA.

The MOF production cost is the sum of the annualised Capital Cost Expenditure (CAPEX), consumables cost, and operating labour (Table 4). The CAPEX for the MOF production is annualised according to the following equations:

$$Annualised\ CapEx = \frac{CAPEX}{Annualised\ Facor}$$

$$Annualised\ Factor = \sum_{i=1}^{n}\left[\frac{1}{(1+r)^{n}}\right]$$

Where:

- n is the plant life (25 years in this analysis),
- r is the discount rate (8%).

A standard 25-year plant life is assumed for the MOF production plant discounting purposes.

The Operating Expenditure (OPEX) was obtained directly from Promethean Particles. Labour associated with the MOF production was calculated using the average UK plant operator salary £35,626/yr [1]. The time taken to produce a defined production campaign volume of MOF was provided by Promethean Particles. Conventionally a number of shift teams are required per shift position in a continuous facility. The total labour requirement is therefore calculated as follows:

$$Labour\ cost = \frac{35{,}626\ (annual\ salary)x\ (shift\ teams)x\ (hours)}{8400\ (annual\ operating\ hours)}$$

Table 4: Capital and Operating Costs and Assumptions for a defined production campaign volume of MOF

Parameter	Cost (£)
Process equipment	
Capital cost of MOF plant (reactor, pumps, compressor, tanks, etc.)	Redacted
Annualised (£/batch)	Redacted
Consumables	
MOF Processing and Shaping	Redacted

Transport	Redacted
Chemicals and consumables	Redacted
Electricity costs	Redacted
Total (£/batch)	Redacted
Labour requirement	
No. operators per process step	
Promethean: Reagent preparation	2
Promethean: MOF Production on CFS Rig	2
Promethean: MOF Washing	2
Labour time per process step	
Promethean: Process Step 1	Redacted
Promethean: Process Step 2	Redacted
Promethean: Process Step 3	Redacted
Total man hours	Redacted
Total (£/batch)	Redacted

Comparison to Literature

MOF production is not yet a mature technology. Manufacturing is currently and typically conducted at batch scale using ball mills, leading to high production costs. The MOF used in this project has been identified as a promising material for CO_2 capture under ambient conditions [2]. While several TEAs have been conducted for MOFs for Carbon Capture and Storage (CCS), they are often based on lab-scale production methods [3]. However, small-scale batch processes are significantly more expensive than continuous-flow synthetic methods, such as those employed by Promethean Particles.

Table 5 details a range of sorbent costs available in literature using different cost estimation methods. Notably, the different estimation methods lead to vastly different MOF costs. This is demonstrated for both MIL-120 and mmen-Mg2(dobpdc) as when bulk reagent costs are used in place of lab reagents the production cost is 100-200 times smaller [4,5,6]. Furthermore, a 44-fold cost reduction is observed when comparing bulk reagent-based production costs to those of the commercially available Zeolite 13X [6]. This variation highlights the importance of using high-quality, system-representative data for MOF production cost estimation, as done in this project.

The estimated production cost for the MOF in this work – at pilot scale, not larger, industrial scale – is comparable to a relevant existing literature estimate [6]. Promethean anticipates the selling price could be reduced significantly when increasing production from the current pilot-scale to commercial scale. This projection is supported by the observed 44-fold reduction in Zeolite 13X costs from the bulk chemical supply costs and literature yields (£66/kg, Table 5) to the industrial scale cost (£1.5/kg, Table 5).

A sensitivity analysis has been conducted to assess the impact of current and projected production costs.

Table 5: Sorbent costs from literature. Costs have been translated onto a £ basis using exchange rates of: £1 = €0.84 and £1 = $0.82.

Sorbent	£/kg sorbent	Reference
Lab Reagent Prices		
MIL-120	2392	[3]
mmen-Mg2(dobpdc)	4781	[3]
Bulk chemical supply costs and literature yields		
MIL-120	11	[4]
mmen-Mg2(dobpdc)	41	[5]
Zeolite 13X	66	[6]
UTSA-16	196	[6]
Industrial		

Zeolite 13X	1.5	[6]

CAPEX

In the previous TEA report the Fixed Capital Investment (FCI) was calculated using the Hand Method to translate Free-on-Board (FoB) costs to installed costs [7]. However, since this estimate, the costs for minor equipment costs have been provided by Promethean. As such, this has been revised to more accurately represent the installed costs by using the summation of the major and minor equipment costs. This change has revised the Inside the Battery Limit (ISBL) CAPEX for the pilot carbon capture rig.

The ISBL is used to calculate the Outside Battery Limit (OSBL) cost (i.e., outbuildings, offices etc.), contingency, and working capital costs. These are collectively used to calculate the Fixed Capital Investment (FCI) and Total Capital Investment (TCI) used in the investment analysis using the parameters presented in Table 6.

Table 6: Fixed Capital Cost Model Assumptions

Economic Parameters	Value	Data Quality	Model Impact	Uncertainty
Cost basis year	2024	High	Low	Low
OSBL	25% of ISBL	High	Low	Low
Contingency	10% of ISBL	High	Low	Low
FCI	ISBL + OSBL + Commissioning	High	Low	Low
Working Capital	10% of ISBL + OSBL	High	Low	Low
TCI	FCI + Working Capital	High	Low	Low
Location Factor	1 (Costs given for UK location)	High	Low	Low

OPEX

Fixed operating costs are costs that are required to be paid independent of the plant being operational, these include labour costs, salary overheads, maintenance, rent of land etc. The parameters used to estimate these for the pilot plant are presented in Table 7 [7].

Table 7: Fixed operating cost parameters

Parameter	Assessment Basis	Unit (Basis)
Maintenance	3	% of ISBL
Property taxes & insurance	1	% of ISBL
Rent of land/buildings	1	% of FCI
General plant overhead	65	% of total labour + maintenance
Allocated environmental charges	1	% of FCI

Specific labour considerations for the pilot MOF capture system have been excluded from this analysis. This is because the capture plant is designed as a retrofit to an existing facility, allowing it to be operated by the current workforce. Additionally, the pilot facility is small, with a design CO2 capture capacity representing less than 0.005% total CO2 emissions from the test site. Including dedicated labour costs for such a small system would disproportionately inflate costs, overshadowing other key cost drivers and performance targets for the pilot system.

Variable operating costs refer to the costs associated with the plant operation. For the capture plant these include electricity, the MOF, and wastewater treatment.

Investment Analysis

The parameters used for the investment analysis and production cost estimation are outlined in Table 8. A 25-year plant lifetime has been assumed for the pilot plant. This approach aligns with the conventions of TEA and ensures that the results are comparable with existing CCS studies.

Table 8: Investment analysis parameters

Economic Parameters	Value	Data Quality	Model Impact	Uncertainty
Discounted Rate of Return (r)	8%	Medium	Medium	Medium
Corporation Tax	25%	High	Low	Low
Linear depreciation	10 years	High	Low	Low
Annual inflation	2%	High	Low	High
Plant Life (n)	25 years	Medium	Medium	Medium

Pilot Data

Pilot data was collected using the pilot CO2 capture rig, and a summary of the findings from these trials, and data used in the TEA from these trials, is outlined in the following section.

Rig Capacity

The original rig design basis was to process flue gas of a given flow rate. However, during early flue gas trials it was found that the incoming flue gas temperature was significantly lower than expected, or designed for, so resulted in challenges within the capture system operation. To compensate for this, and ensure safe operation, changes were undertaken which meant the inlet flue gas flowrate was reduced. Consequently, the CO_2 flowrate entering the rig was reduced and the design capture capacity is not demonstratable using the current set up. However, to demonstrate the systems potential a hypothetical case is presented considering this capture rate assuming the rig could be used at full capacity.

Competitive Adsorption With Water

The competitive adsorption of water during CO2 capture reduces the number of active binding sites and is a known issue for CO2 adsorption processes [11]. In addition, water can interfere with the chemical stability of some MOFs by either permanently terminating the sites or breaking the network structure via hydrolysis [12]. During pilot trials the MOF demonstrated water uptake in addition to CO2. This caused problems with regeneration where the system was unable to adequately remove the adsorbed water due to design limitations. In existing TEA and LCA studies molecular sieve units have been considered prior to the MOF adsorber to dehydrate the flue gas [13]. This pre-treatment would provide dry flue gas to the MOF potentially removing the observed issues. However, pilot trials using a dehydration unit prior to the MOF capture system are required to verify this.

Pilot Data Use

The first pilot adsorption trial using fresh MOF is used as the basis for the TEA. It is assumed that the flue gas would be dried prior to entering the adsorber to allow for vacuum regeneration which was found to adequately remove the adsorbed CO2 during the trials. Note that due to the absence of trial data on the use of dehydration prior to adsorption, the capital and operating expenditure associated with this has not been considered in the TEA.

Under cyclic conditions each column would operate in adsorption mode up to breakthrough. This amount of CO2 would then be desorbed while the other column enters adsorption mode. The quantity of CO2 adsorbed until breakthrough, time to reach breakthrough, and desorption time to desorb this quantity of CO2 is taken directly from the pilot trial data. These parameters are used to calculate the adsorption capacity (mmol/g), adsorption cycle time (minutes), desorption cycle time (minutes), and extrapolate to the total capture per annum (tnCO2/yr). The electricity usage across the adsorption and desorption cycle is used to calculate the electricity demand per annum.

Design Capacity

Based on the adsorption capacity and cycle time from the pilot trials the current annual CO2 uptake is estimated. To operate at the design capacity, the flue gas flowrate would need to be increased to the design flowrate along with other changes. At present the pilot rig components are oversized for the flue gas throughput.

To demonstrate the potential of the system a ‘Design Capacity Case’ has been modelled which assumes the design flowrate of flue gas is processed.

The adsorption and desorption cycle times and electricity use for this case have been calculated pro-rata using the pilot data based on the cycle time. No adjustment to electricity usage has been made for the flue gas flowrate as the equipment is currently oversized and no pilot data is available at this operating capacity. Further pilot tests need to be undertaken to confirm if the proposed annual capacity is achievable at the design capacity flowrate and what the corresponding adsorption capacity, electricity use, and cycle time would be.

Capture Cost

The current pilot performance results in a cost higher than the UK emission trading scheme cost of £83/tnCO2 [15] and EU carbon permits of £67/tnCO2 [16]. Increasing the uptake capacity has a marked difference on the capture cost, bringing it closer to the UK emission trading scheme cost. It further demonstrates the potential of the system provided that this target is achieved with further testing and verification of MOF cycling. Note that additional capital and operating expenditure would be required if a dehydration unit were to be installed to facilitate MOF cycling, this has the potential to increase the capture costs.

Sensitivity Analysis

A sensitivity analysis was conducted using the design capacity as the baseline demonstrating the impact of various performance variables. Notably, the adsorption capacity and cycle time are the most influential variables on the capture cost. This highlights the importance of verifying if an increased annual capacity is achievable with further pilot test data and demonstrating MOF cycling in future pilot trials.

Literature Comparison

To contextualise the TEA outcomes the following section provides a comparison between CCS costs for MOF systems and a conventional MEA capture system. Achieving the design capacity brings the costs in line with comparative literature estimates (Table 9). However, further optimisation of the capture system is required to demonstrate the cycle time and adsorption capacity to realise this target.

Table 9: CO2 capture costs from literature. Costs have been translated onto a £ basis using exchange rates of: £1 = €0.84 and £1 = $0.82.

Sorbent	£/tnCO21	Reference
Zeolite 13X	40.82	[13]
UTSA-16	52.16	[13]
IISERP MOF2	25.87	[13]

TA-MOF343 (no heat recovery)	168.51	[17]
TA-MOF343 (35% heat recovery)	78.23	[17]
UTSA-16	74.62 - 120.56	[18]
MEA	62.46	[19]

Conclusions

This report provides a full TEA of the CCS pilot plant installed at the test site. It includes updates made for the CAPEX and OPEX for MOF production, and CAPEX and OPEX for the CCS pilot plant. The MOF production cost for manufacturing at pilot-scale was determined and Promethean anticipates this could be reduced significantly at industrial scale. This level of reduction is supported by literature which demonstrates a significant decrease in manufacturing costs when transitioning to industrial scale.

The pilot capture plant is designed as a retrofit operating at a capacity less than 0.005% of the test site’s total CO2 emissions. As such, specific labour considerations were excluded to prevent these costs overshadowing other key cost drivers and performance targets for the pilot system.

Pilot tests were conducted on a reduced flow of flue gas rather than the design capacity due to a sequence of events that transpired as a result of the incoming flue gas temperature being significantly lower than expected. As such the total CO2 flowrate to the rig made the capture target unattainable on the current system. Furthermore, the competitive adsorption of water was found to cause challenges that limited data collection. As other CO2 adsorption systems commonly have molecular sieve units installed to dehydrate the gas prior to CO2 capture it was assumed this could be retrofitted, and data for the TEA was still able to be obtained prior to the observed challenges. However, pilot trials are required to verify that dehydration of the flue gas enables MOF regeneration. Due to the absence of trial data the capital and operating expenditure associated with dehydration, this has not been considered in the TEA.

Additional pilot data is needed to confirm the feasibility of the proposed annual capture capacity, and other associated factors. It should also be noted that any additional capital and operating expenditure associated with dehydrating the flue gas to facilitate MOF cycling may increase the capture cost calculated in this work.

The sensitivity analysis highlighted both adsorption capacity and cycle time as the most influential variables on the capture cost, thereby emphasising the need to verify if the capacity is achievable through future pilot trials.

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