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# INTERNATIONAL MASTER'S PROGRAMME IN ENERGY AND GREEN HYDROGEN (IMP-EGH)

Speciality: Economics/Policies/Infrastructures and Green Hydrogen Technology

**Topic:**

Modelling the cost structure and value chain of e-methanol production using solid sorbent Direct Air Capture in Arid regions

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# **Dedication**

<span id="page-1-0"></span>To my parents, who have been my source of inspiration and motivation, I dedicate this work with gratitude and love. I dedicate this work with respect and admiration to my supervisor, Prof. Dr. Maria Mercedes Movsessian, who has been my mentor and advisor. I dedicate this work with hope and optimism to all the visionaries and innovators striving for a greener and cleaner future.

# **Declaration of authorship**

<span id="page-2-0"></span>I, Abraham Josaphat Miflinso Yehouenou,

declare that this thesis and the work presented in it are my own and have been generated by me as the result of my original research.

I do solemnly swear that:

1. Where I have consulted the published work of others or myself, this is always clearly attributed;

2. Where I have quoted from the work of others or myself, the source is always given. This thesis is entirely my work, except for such quotations;

3. I have acknowledged all major sources of assistance;

4. Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;

5. None of this work has been published before submission;

6. During the preparation of this work, I used Quillbot, Wordtune and Grammarly to edit the writing of the thesis. After using this tool/service, I reviewed and revised the content as needed and took full responsibility for the content.

Date: 14/09/2023 Signature:

Abraham J. M. Yehouenou

# **Acknowledgement**

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### **Abstract**

<span id="page-5-0"></span>Since  $CO<sub>2</sub>$  is the primary greenhouse gas causing global warming,  $CO<sub>2</sub>$ -free solutions like emethanol enable the energy transition. E-methanol is renewable and carbon-negative by extracting CO<sub>2</sub> from the air via Direct Air Capture sorbent. While e-methanol is environmentally beneficial, is it economically feasible? This research examined the cost structure and value chain for two e-methanol production scenarios. Scenario 1 uses solid sorbent DAC for  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$ to generate syngas via co-electrolysis with solid oxide electrolysis cells (SOEC), then methanol by CO hydrogenation. Scenario 2 is direct  $CO<sub>2</sub>$  hydrogenation using DAC  $CO<sub>2</sub>$  and PEM hydrogen. Analysing inputs/outputs showed Scenario 1 consumes fewer raw materials and energy with better efficiency. SOEC Syngas Scenario 1 has a 0.63€/kg levelized cost, 50% lower than the 1.26 €/kg for PEM hydrogen Scenario 2. Detailed cost structure analysis revealed syngas/hydrogen, electricity, SOEC capital, and DAC capital/sorbent costs as key drivers. Sensitivity analysis showed 16% lower Scenario 1 methanol cost with projected 2050 SOEC capital reductions, 10% lower with DAC capital reductions, and 33% lower with electricity reductions.

Keywords: Syngas, e-methanol, hydrogen, cost structure, sorbent

### **Résume**

<span id="page-6-0"></span>Le CO<sub>2</sub> étant le principal gaz à effet de serre à l'origine du réchauffement climatique, les solutions sans CO<sub>2</sub> telles que l'e-méthanol favorisent la transition énergétique. L'e-méthanol est renouvelable et ne produit pas de carbone en extrayant le  $CO<sub>2</sub>$  de l'air par le biais d'un sorbant de capture directe de l'air. Si l'e-méthanol est bénéfique pour l'environnement, est-il économiquement réalisable ? Cette étude a examiné la structure des coûts et la chaîne de valeur de deux scénarios de production d'e-méthanol. Le scénario 1 utilise un sorbant solide DAC pour le CO<sub>2</sub> et le H<sub>2</sub>O afin de générer du gaz de synthèse par co-électrolyse avec des cellules d'électrolyse à oxyde solide (SOEC), puis du méthanol par hydrogénation du CO. Le scénario 2 est l'hydrogénation directe du CO<sub>2</sub> à l'aide du DAC CO<sub>2</sub> et de l'hydrogène PEM. L'analyse des intrants et des extrants a montré que le scénario 1 consomme moins de matières premières et d'énergie avec une meilleure efficacité. Le scénario 1 de SOEC syngas a un coût levé de 0,63 €/kg, soit 50 % de moins que les 1,26 €/kg du scénario 2 de l'hydrogène PEM. L'analyse détaillée de la structure des coûts a révélé que le gaz de synthèse/hydrogène, l'électricité, le capital de la SOEC et le capital du DAC/les coûts des absorbants étaient les principaux facteurs. L'analyse de sensibilité a montré que le coût du méthanol du scénario 1 était inférieur de 16 % avec les réductions de capital SOEC prévues pour 2050, de 10 % avec les réductions de capital DAC et de 33 % avec les réductions d'électricité.

Mots-clés : Gaz de synthèse, e-méthanol, hydrogène, structure des coûts, sorbant.

## **Acronyms and abbreviations**

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# **Chapter I: Introduction**

#### <span id="page-12-1"></span><span id="page-12-0"></span>1. Background and Context

For more than a decade, it has been no secret that the climate crisis we are experiencing is primarily due to our fossil fuels. Under the Paris Agreement, countries committed to limiting global warming and keeping the average temperature below 2 degrees Celsius, with the aim of bringing it down to 1.5 degrees Celsius. An alternative to fossil fuels is therefore the mitigation tool that the Nations are looking for.

One of the promising solutions is e-methanol, an energy carrier and chemical feedstock that could aid in the transition towards a carbon-neutral economy (Emebu et al., 2023). Also denoted as MeOH, methanol is one of the crucial industrial materials. Its increasing demand is due to its promising characteristics as an energy vector leading to increasing interest in the concept of a future methanol economy (Jarvis & Samsatli, 2018). Methanol is traditionally produced with synthesis gas (syngas), a mixture of  $CO$ ,  $CO<sub>2</sub>$  and  $H<sub>2</sub>$  from steam methane reforming resulting in high  $CO<sub>2</sub>$  emissions (Biswal et al., 2022). In recent years, the Renewable methanol or e-methanol concept has emerged resulting in the use of carbon captured and hydrogen. E-methanol couples the benefits of harmful carbon emission reduction and positive water management when produced using  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$  captured from direct air capture and hydrogen or syngas from electrolysis using renewable energy. This route provides an option for storing renewable energy in a chemical form that is compatible with the current energy infrastructure, while simultaneously addressing the issue of  $CO<sub>2</sub>$  emissions (Deka et al., 2022; International Renewable Energy Agency, 2021) and water scarcity. This is especially relevant in industries and transport sectors where direct electrification is challenging.

While e-methanol presents significant environmental benefits, its economic feasibility is still to be proved. The cost components like capital investment, operational expenses, and maintenance are factors that could impact its market viability (Deka et al., 2022). Its production from  $CO<sub>2</sub>$ captured and hydrogen is studying for a couple of years and the major costs are hydrogen and energy costs (Nizami et al., 2022). The emergence of Solid Oxide Electrolysis Cell with the capacity of co-electrolysis is seen as a game changer for e-methanol production (Lonis et al., 2021) primarily because of the high efficiency of SOEC. It is therefore crucial to develop an indepth understanding of the cost structure and value chain of e-methanol production using  $CO<sub>2</sub>$ from solid sorbent direct air capture and syngas from SOEC co-electrolysis.

### <span id="page-13-0"></span>2. Problem Statement

Despite its potential for mitigating climate change, the production of e-methanol, particularly through the utilisation of  $CO_2$  capture and  $CO_2/H_2O$  co-electrolysis with Solid Oxide Electrolysis Cell, faces significant challenges.

Firstly, the technology for capturing  $CO<sub>2</sub>$  from the air is still emerging (Baptie, 2021), resulting in high capture costs. Moreover, sorbent cost for Direct Air capture has lower efficiency and different performance under different climate conditions (Husk & Wenz, 2022). Secondly, the SOEC process, while efficient, is still on a lab scale with operational and cost-related uncertainties, thus resulting in vague cost structures compared to alkaline and proton exchange membrane electrolysers (Anghilante et al., 2018; Liu et al., 2023). Co-electrolysis with SOEC is not well studied and can lead to further cost implications (Jambur, 2022).

Moreover, the value chain for e-methanol production by this process is complex, requiring meticulous coordination across multiple stages since most feedstocks are produced from the same process. A complete production plant from the energy generation to methanol synthesis including  $CO_2$  capture and  $CO_2/H_2O$  co-electrolysis does not need feedstock supply and transportation in its value chain. This complex scheme could present potential bottlenecks for large-scale production.

Modelling and understanding the cost structure and value chain of this manufacturing process is therefore essential to identify areas for improvement, challenges and potential solutions. This level of understanding is required to drive research, investment, policy formulation and implementation in the e-methanol production sector.

Without a thorough understanding of these costs and the dynamics of the value chain, there is a risk that e-methanol's potential as a sustainable alternative to methanol from fossil fuels will not be realised. This could ultimately impede progress towards the global energy and climate change ambitions of the Paris Agreement.

# <span id="page-13-1"></span>3. Scope of Study

This study focuses on e-methanol production using  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$  captured from Direct Air Capture (DAC) and Syngas from co-electrolysis of Solid Oxide Electrolysis Cells (SOEC) in arid regions proposed by the DryHy project. It will detail the production process and technical requirements, analyse the cost structure, find the cost drivers, and evaluate the production value chain and the value added in each stage of the production. It will also consider the use of

hydrogen from a proton exchange membrane (PEM) electrolyser for e-methanol production as a second scenario to evaluate and compare the value added in the chain of production with SOEC. The study will focus only on the production value chain and will not involve transport and distribution as well as end use. The study won't delve into environmental impact, life cycle analysis, or market and policy considerations. It will only provide some general policy recommendations that could make viable such process.

### <span id="page-14-0"></span>4. Research objectives

The overall objective of this study is to model and understand the cost structure and value chain of e-methanol production from solid sorbent direct air capture and solid oxide electrolysis cells in arid regions.

More specifically, the research aims to:

- **Determine the production process for each step**: Describe the detailed steps of the emethanol production process, and assess the technical requirements, the technology readiness level, the efficiency of the technologies used, including the coadsorption/desorption of  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$ , syngas production, and methanol synthesis.
- **Determine the inputs and outputs of each stage**: Identify and quantify the valuable raw materials and outputs involved in each stage of production and their interconnection in the production chain.
- **Analyse the cost structure**: estimate the costs relating to each stage of the production process, including investment costs, operational costs, maintenance costs and raw material costs.
- **Analyse the value chain**: Identify all stages of production and study the interconnections between them, determine the added value at each stage and detect potential bottlenecks and critical dependencies in the value chain.
- <span id="page-14-1"></span>5. Research Questions
- What are the detailed steps of the e-methanol production process and the technical considerations for implementing the technologies involved?
- What are the useful inputs and outputs at each stage and how are they linked to the production chain?

- What are the costs associated with each step of the e-methanol production process, and the cost drivers?
- What are the different stages of the e-methanol production value chain and what are the value added at each stage?
- <span id="page-15-0"></span>6. Hypothesis
- E-methanol production process involved Renewable Energy generation,  $CO<sub>2</sub>$  and Water capture, Electrolysis and CO<sub>2</sub> hydrogenation;
- The main inputs and outputs of each stage are renewable electricity, water,  $CO<sub>2</sub>$ , syngas, methanol, and waste heat;
- The cost structure of e-methanol is dominated by the electricity cost followed by the capital expenditure of Direct Air capture;
- The value chain of e-methanol production consists of four main stages: energy generation, air capture, electrolysis and synthesis, and each stage adds value by transforming low-value inputs into high-value outputs.

## Chapter II: Literature Review

- <span id="page-16-2"></span><span id="page-16-1"></span><span id="page-16-0"></span>1. Overview of methanol synthesis and e-methanol
	- 1.1. Methanol and e-methanol

Methanol has special properties that set it apart from other renewable fuels. Already known throughout the world as an essential chemical compound for industry, it has also established itself as a carrier of hydrogen, as a fuel (International Renewable Energy Agency, 2021) and more generally as a raw material for flexible chemistry and energy (Chen et al., 2021). In recent decades, this has even led to the prospect of a future methanol economy (Lonis et al., 2021). Indeed, methanol can be easily used, transported, and stored without major modification of existing infrastructures (vehicle engines, fuel distribution and transportation systems). On the other hand, the transition to a hydrogen economy with mass production and use of pure hydrogen will lead to a revolution in fuel infrastructure (Deka et al., 2022b). Methanol is a very interesting means of storing energy, since it is a carrier with high energy density, both in weight and in volume, which does not require storage at high pressure, given that its boiling point at ambient pressure is about 65°C.

In 2015, global methanol demand was around 70 million tonnes. About 40% of this demand concerns energy applications (Deka et al., 2022b). Typically, methanol is produced from fossil fuels by steam reforming of methane or by gasification of coal, but it can also be produced by other improved processes such as catalysed hydrogenation of CO (Lonis et al., 2021). With growing concerns about climate change due to  $CO<sub>2</sub>$  emissions, the development of innovative systems for the production and use of renewable methanol or e-methanol, for example methanol produced from renewable energy sources and recycling or capture of  $CO<sub>2</sub>$ , is an attractive option for reducing the environmental impact of fossil fuels consumed in the energy, transport, and industrial sectors. Methanol is often used as a raw material for petrochemicals (formaldehyde, acetic acid, propylene, ethylene, etc.), to produce heat or steam in the maritime and road transport sectors (Lonis et al., 2021). On the other hand, due to the gradual increase in the activity of renewable energy, the major contribution of energy storage is fundamental to increasing the overall penetrability, usability, and orchestration capacity of renewable energy. In this context, methanol as an energy carrier can contribute to solving the main problems related to energy storage.

# <span id="page-17-0"></span>1.2. Methanol applications

1.2.1. Chemical Sector

Methanol is one of the most important basic chemicals, with annual global demand reaching 98 million tonnes in 2019. It is widely used to produce hundreds of everyday industrial chemicals and consumer products. About two-thirds of methanol is used to produce other chemicals like formaldehyde, acetic acid, methyl methacrylate (MMA), and olefins through the methanol-toolefins (MTO) route. Formaldehyde is the largest chemical derivative, mainly used to produce resins and adhesives. MTO has seen tremendous growth in the past decade in China to produce polyethylene and polypropylene plastics. MTO now accounts for about 25% of global methanol consumption. Methanol is also used to produce methyl tert-butyl ether (MTBE), an oxygenate additive blended with gasoline, and biodiesel through transesterification of plant oils/animal fats(Deka et al., 2022b).

In the long term, renewable methanol could replace most petroleum-based chemicals and materials. This would facilitate the transition to a sustainable circular green economy in the chemical sector(Deka et al., 2022b).

# 1.2.2. Transport Sector

About 31% of methanol is used as a fuel in the transport sector. China has promoted methanol as an alternative transport fuel to reduce oil imports. Methanol has a high-octane rating and can be blended with gasoline or used directly in flex-fuel vehicles. It allows for higher engine compression ratios and efficiency. Blends up to M15 can be used in regular cars; higher blends like M85/M100 need flex-fuel vehicles. It is used in taxis, cars, buses, trucks, and heavy-duty vehicles in China and is being introduced in other countries. Methanol fuel standards exist or are being developed in China, Israel, Italy, India, and others(Roode-Gutzmer et al., 2019).

Methanol is also emerging as a clean marine fuel for ships and ferries. It reduces PM, SOx and NOx emissions by >95%, 99% and 60-80% respectively compared to heavy fuel oil. Methanol bunkering infrastructure is readily available in 100+ ports. DME produced from methanol is a diesel substitute. Methanol can also be used in advanced hybrid and fuel cell vehicles, reformed on-board to hydrogen to power fuel cells(Roode-Gutzmer et al., 2019).

## 1.2.3. Industrial Sector

Methanol is used as a fuel in industrial boilers and kilns. Over 1,000 industrial boiler units in China use methanol for heat and steam generation. It can also be used to produce electricity in gas turbines, fuel cells, and other engines. Around 2 million tonnes of methanol were used for power/heat generation in China in 2018(Chen et al., 2021; Roode-Gutzmer et al., 2019).

### 1.2.4. Other Uses

Methanol has some niche applications in other sectors, such as wastewater treatment, refrigeration, antifreeze, explosives, and cosmetics. Methanol is also used as a feedstock to produce methyl tert-butyl ether (MTBE) and methyl methacrylate (MMA), which are used as gasoline additives and acrylic plastics, respectively. Global methanol demand is projected to continue increasing, reaching over 500 million tonnes per year by 2050. The growth will have to increasingly shift to renewable methanol to reduce emissions and facilitate the transition to a sustainable circular economy(Chen et al., 2021).

### <span id="page-18-0"></span>1.3. Methanol markets

Global demand for methanol has undergone robust growth over the past decade, nearly doubling to reach approximately 98 million tonnes in 2019 (Chen et al., 2021). China dominates the market, accounting for 55 million tonnes (over half) of global consumption in 2018, driven by major growth applications including olefins production and gasoline blending (Deka et al., 2022b). Total worldwide production capacity now stands at around 150 million tonnes per annum, with the majority still derived from non-renewable fossil fuel feedstocks - approximately 65% from natural gas and 35% from coal (Deka et al., 2022b). Only a minor share of about 0.2% is currently produced renewably from biomass and waste sources. Average European market pricing has fluctuated between USD 200-400 per tonne over the past decade, while estimates for production costs range from USD 100-250 per tonne for natural gas and USD 150-250 per tonne for coal-based production (Roode-Gutzmer et al., 2019). Market demand is projected to continue rising significantly, potentially reaching over 120 million tonnes by 2025 and 500 million tonnes by 2050, highlighting the need for greater adoption of renewable methanol production pathways to support sustainable growth.

# 1.4. Methanol production and feedstocks

<span id="page-19-0"></span>Methanol production utilises carbon dioxide  $(CO_2)$  as a key feedstock component. Traditionally, methanol is produced from fossil fuel sources like natural gas, coal, and crude oil through processes like steam methane reforming and coal gasification (Lonis et al., 2021). However, interest is growing in renewable  $CO<sub>2</sub>$  sources to reduce greenhouse gas emissions. This literature review categorises and examines methanol feedstocks by CO<sub>2</sub> source.

# 1.4.1. Fossil Fuel-Derived CO<sup>2</sup>

Most methanol today uses  $CO<sub>2</sub>$  from fossil fuel processing. Steam reforming or gasification of natural gas and coal produces syngas containing  $CO<sub>2</sub>$  and CO. This syngas is then catalytically converted to methanol. Coal gasification provides  $67\%$  of  $CO<sub>2</sub>$  for China's methanol industry (Roode-Gutzmer et al., 2019). Natural gas reforming accounts for 33% of global CO2 feedstocks (Lonis et al., 2021).

# 1.4.2. Waste-Derived CO<sub>2</sub>

Municipal solid waste gasification and biogas production yield  $CO<sub>2</sub>$  suitable for methanol synthesis. Companies like Enerkem and CRI utilise waste-derived  $CO<sub>2</sub>$  at commercial scales, reducing lifecycle emissions by over 90% (Roode-Gutzmer et al., 2019). Waste gasification appears more scalable and cost-effective than other renewable CO2 sources currently(Lonis et al., 2021).

# 1.4.3. Industrial  $CO<sub>2</sub>$  Streams

Captured CO<sub>2</sub> from industrial point sources like steel manufacturing or ethanol production can be used. This route for renewable methanol production is the hydrogenation of recycled carbon dioxide using hydrogen produced from water electrolysis powered by renewable electricity (Lonis et al., 2021). This process allows carbon dioxide emissions to be captured and recycled rather than released into the atmosphere.

# 1.4.4. Atmospheric CO<sup>2</sup>

The process of using  $CO_2$  captured from the atmosphere and green hydrogen or syngas to produce e-methanol is a way of converting renewable energy and carbon dioxide into a liquid fuel that can be used as a substitute for fossil-based methanol. The process involves two main steps: capturing CO<sup>2</sup> from the atmosphere and synthesising it with hydrogen or syngas to methanol.

This process can be considered carbon-negative, as it removes  $CO<sub>2</sub>$  from the atmosphere and converts it into a useful product(International Renewable Energy Agency, 2021).



Figure 1: E-methanol production methods Source: (International Renewable Energy Agency, 2021)

- <span id="page-20-1"></span><span id="page-20-0"></span>2. Electrolysis of water to hydrogen followed by catalytic methanol synthesis.
	- 2.1. Literature review on the technologies involved and economics.
		- 2.1.1. Direct Air Capture and Sorbent

<span id="page-20-2"></span>Direct air capture (DAC) is a technology that captures carbon dioxide  $(CO<sub>2</sub>)$  directly from the ambient air (Kuru et al., 2023). This contrasts with carbon capture and storage (CCS), which captures  $CO<sub>2</sub>$  from point sources such as factories or power plants (Kuru et al., 2023). DAC reduces the carbon dioxide concentration in the atmosphere, making it a promising technology for mitigating climate change.

There are two types of DAC: solid DAC (S-DAC) and liquid DAC (L-DAC). S-DAC or lowtemperature DAC (LT-DAC) is based on solid sorbents that capture  $CO<sub>2</sub>$  from the air. In contrast, liquid DAC or high-temperature DAC (HT-DAC) involves passing air through a chemical solution to remove carbon dioxide. In terms of water capture, solid DAC has the added benefit of capturing water from the air, which can be used for other purposes. Most commercial techniques require large fans to push ambient air through a filter. The captured  $CO<sub>2</sub>$  can then be sequestered or utilised to produce carbon-neutral fuel (Fasihi et al.,2019).

[Figure 2](#page-21-0) shows the differences between Low-temperature Direct Air Capture and Hightemperature Direct Air Capture and the companies using them.



<span id="page-21-0"></span>Figure 2: Companies active in the field of CO<sub>2</sub> DAC. Abbreviations: high temperature, HT, low temperature, LT, moisture swing adsorption, MSA, temperature swing adsorption, TSA.

Source: (Fasihi et al., 2019)

There are two major solid-sorbent Direct Air Capture based on their regeneration method. Temperature Swing Adsorption (TSA) Direct Air Capture uses heat to release  $CO<sub>2</sub>$  from the sorbent material, usually a solid amine or a metal-organic framework (MOF). The sorbent material is exposed to the air at low temperatures and high humidity, where it adsorbs  $CO<sub>2</sub>$  along with H<sub>2</sub>O. Then, the sorbent material is heated to a high temperature and low humidity, where it desorbs  $CO_2$ . The core advantage of TSA DAC is it has  $CO_2$  selectivity ranging from 50 to 90% and still works under high temperatures and low humidity.

# 2.1.2. Economics of Solid sorbent Direct Air Capture

Most articles regarding DAC focus on technical parameters, and only a few have conducted economic estimations. All reviewed economic specifications and costs are summarised in [Table](#page-22-0)  [1.](#page-22-0)

<span id="page-22-0"></span>

<b>Sorbent</b>	<b>Sorbent</b> cost	Capex $\epsilon/t$	<b>Opex</b> $\frac{0}{0}$	Life time	El. <b>Demand</b> $KWh_{el}/t$	El. <b>Price</b> E/KWh	Heat source/ demand $KWh_{th}/t$	Cost of capture $\epsilon/t$	<b>Reference</b>
Amine- <b>based</b>				25	200-300		Waste heat/1500- 2000	75	Climeworks 2018
				$\overline{\phantom{a}}$	150-260		1170-1410	$100 -$ 550	Ping et al. 2018, reported by (Fasihi et al., (2019)
<b>MOF</b>	15	140	$\overline{\phantom{a}}$	25		0.06		221	(Sinha et al., 2017)
		730	$\overline{4}$	20	250	$\blacksquare$	Waste heat Heat pump:1750	133/155	(Fasihi et al., 2019)
	15			25		0.06	geothermal	205	(McQueen et al., 2020)
Lewati VP <sub>OC</sub> 1065	30					0.1	Heat pump	308	(Bos et al., 2020a)
Lewati VP OC 1065	30	730	$\overline{\mathbf{4}}$	25	250	<b>Solar</b> <b>PV</b>	<b>Waste</b> heat		This work

Table 1: Economics parameters of solid direct air capture as reported in the literature.

# 2.1.3. Green Hydrogen Production

Green hydrogen production is the process of producing hydrogen using renewable energy sources, such as wind or solar power, and water through electrolysis. Electrolysis is a chemical process that uses electricity to split water molecules into hydrogen and oxygen. Electrolysers are the critical technology used in green hydrogen production. They are devices that use electricity to split water into hydrogen and oxygen molecules (*International Energy Agency*., 2022). The primary reaction involved in that process is as follows:

$$
2H20 == > 2H2 + 02
$$

Several types of electrolysis technologies are used in green hydrogen production, including alkaline electrolysis, proton exchange membrane (PEM) electrolysis, and solid oxide

electrolysis. Each technology has advantages and disadvantages, and the choice of technology depends on cost, efficiency, and scalability.

- Alkaline electrolysers use a liquid alkaline solution as the electrolyte and nickel electrodes(*PEM vs. Alkaline Electrolysis*, 2021). They are the most mature and widely used technology, with low capital and maintenance costs. However, they have lower efficiency, slower response time, and higher sensitivity to impurities than other types of electrolysers (*International Energy Agency*., 2022).
- PEM electrolysers use a solid polymer membrane as the electrolyte and platinum electrodes. They have higher efficiency, faster response time, and lower sensitivity to impurities than alkaline electrolysers. They can also operate at higher pressures and produce higher-purity hydrogen(*PEM vs. Alkaline Electrolysis*, 2021). However, they have higher capital and maintenance costs due to using expensive materials (*International Energy Agency*., 2022).
- Solid oxide electrolysers use a ceramic material as the electrolyte and metal or ceramic electrodes. They operate at high temperatures (around  $800^{\circ}$ C) and can use steam or  $CO<sub>2</sub>$ as the feedstock. They have the highest efficiency and can produce syngas (a mixture of hydrogen and carbon monoxide) in addition to hydrogen. However, they have high capital and operating costs, long start-up time, and lower durability than other electrolysers(Liu et al., 2023).

# 2.1.4. Direct  $CO<sub>2</sub>$  hydrogenation

In the direct  $CO_2$ -to-methanol electrolysis pathway, carbon dioxide  $(CO_2)$  and hydrogen  $(H_2)$  are converted into methanol (CH3OH), a liquid fuel and chemical feedstock. The technology to produce methanol is thus already mature and very similar to the one used in traditional fossil fuel-based plants. The plant will produce e-methanol with > 99% yield and selectivity. The reaction of CO<sub>2</sub> with hydrogen is exothermic (releases energy), and the heat of the reaction can be used to provide other plant services(International Renewable Energy Agency, 2021). Reported by-products during methanol synthesis include  $H_2$ , CO, and HCOOH, which are subsequently purified via pressure swing adsorption and distillation stages and recovered for sale.

### 2.2. Cost Structure

<span id="page-24-1"></span>According to a review by the International Renewable Agency, the cost of e-methanol depends to a large extent on the cost of hydrogen and  $CO<sub>2</sub>$ . The cost of  $CO<sub>2</sub>$  depends on the source from which it is captured, e.g. from biomass, industrial processes, or DAC. The cost of making emethanol today depends on where the  $CO<sub>2</sub>$  comes from. If it comes from biomass costing USD 10-50/t, then e-methanol costs USD 800-1 600/t. If it comes from DAC, which costs USD 300- 600/t, then e-methanol costs USD 1 200-2 400/t. The cost of green hydrogen, which is also needed for e-methanol, will decrease as renewable power and electrolysers become cheaper and more efficient (International Renewable Energy Agency, 2021).

Table 2: Methanol through  $CO<sub>2</sub>$  from DAC only

<span id="page-24-0"></span>

		2018	2030	2050
Cost of CO2 from DAC (USD/t $CO2$ )	$300 - 600$	150-300	$50-150$	
<b>Cost of methanol</b>	With no carbon credit	1220-2380	600-1070	290-630
(USD/t MeOH)	With a credit of USD $50/t$ CO <sub>2</sub>	1130-2300	510-980	200-550
	With a credit of USD $100/t$ CO <sub>2</sub>	1040-2210	420-890	120-460

### Source: (International Renewable Energy Agency, 2021)

Bos et al., (2020) present a techno-economic evaluation of renewable methanol production from wind power, water electrolysis, and direct air captured CO2. They assume a wind farm capacity of 100 MW in the Netherlands and a PEM electrolyser operating for 4800 hours annually. The direct air CO2 capture cost is estimated as 200  $\epsilon$ /tonne, using heat pumps for desorption. Methanol synthesis only contributes about 5% of the total capital cost. The levelized cost of methanol is estimated as 800  $\epsilon$ /tonne, considering 0.05  $\epsilon$ /KWh for electricity cost. The results show that electricity cost is the main contributor to the production cost, followed by the capital expenditure of the CO2 direct air capture system, including sorbent material. The methanol synthesis section has a relatively small contribution to the overall cost.

Nizami et al., (2022) performed a techno-economic assessment of renewable methanol production from hydrogen and captured carbon dioxide. They estimated a levelized cost of methanol (LCoM) of 1040 \$/tonne using electricity from the grid and 1669 \$/tonne from photovoltaics and batteries. They identified electricity prices as having the most significant impact, contributing 67-81% to the LCoM.

Sollai et al., (2023) performed a techno-economic assessment of a commercial-scale renewable methanol production plant. Their analysis estimated a levelized cost of methanol (LCoM) of 960

 $\epsilon$ /tonne, more than double the current market price of methanol. In agreement with the other studies, Sollai et al. found the electricity price and electrolyser cost have the most impact on LCoM. The cost of  $CO<sub>2</sub>$  feedstock contributed around 10% to the total production costs.

Finally, a review by (Schmidt et al., 2018) looked at methanol production from  $CO<sub>2</sub>$  and hydrogen via the power-to-liquids pathway. With  $H_2$  produced by water electrolysis using renewable electricity and  $CO<sub>2</sub>$  captured from various sources, the estimated levelized cost of methanol was on average  $\epsilon$ 1.24/kg and highly sensitive to electricity price. The study suggests that electricity prices could reach 2-4  $\epsilon$ cents/kWh by 2050 with increasing renewable energy penetration. This could reduce methanol cost to  $0.5 \, \epsilon$ /kg.

- <span id="page-25-1"></span><span id="page-25-0"></span>3. Electrolysis of water and carbon dioxide to syngas followed by catalytic methanol synthesis.
	- 3.1. Process description
		- 3.1.1. Co-electrolysis with Solid Oxide Electrolysis Cell (SOEC)

 $CO<sub>2</sub>/H<sub>2</sub>O$  co-electrolysis with SOEC for syngas production is a process that uses solid oxide electrolysis cells (SOECs) to convert carbon dioxide and water into a mixture of hydrogen and carbon monoxide, also known as syngas(Dieterich et al., 2020; Jambur, 2022). Syngas can be used as a fuel or feedstock for synthesizing hydrocarbons and other chemicals.

The basic principle of syngas production with SOEC for methanol synthesis is to apply an electric potential across two electrodes separated by a solid oxide electrolyte. The feed gas, which contains  $CO_2$  and  $H_2O$ , is supplied to the cathode, which is reduced to CO and  $H_2$  by gaining electrons from the external circuit. The oxygen atoms are transported through the electrolyte to the anode, oxidising to  $O_2$  by losing electrons to the external circuit. The product gas, which contains CO and H2, is collected from the cathode side(Dogu et al., 2019)

Cathode reactions (Dogu et al., 2019):

 $CO_2 + 2e^- \rightarrow CO + O_2 (1)$  $H_2O + 2e^- \rightarrow H_2 + O_2(2)$ Anode reaction (Dogu et al., 2019):

$$
20_2 \rightarrow 0_2 + 4e^-(3)
$$

The advantages of syngas production with SOEC for methanol synthesis include:

- High energy conversion efficiency: The process can achieve theoretical efficiencies close to 100%, depending on the operating conditions and the cell design (Dieterich et al., 2020).
- Integration with various energy sources: The process can use electricity from renewable sources, such as wind, solar, or geothermal, or from excess power generation, such as nuclear or coal-fired plants (Dieterich et al., 2020).
- Reversibility: The process can operate in both electrolysis and fuel cell modes, depending on the direction of the electric current. This allows for energy storage and conversion in a single device (Dieterich et al., 2020).
- Adaptability: The process can produce syngas with different  $H<sub>2</sub>/CO$  ratios, depending on the feed gas composition and the operating parameters. This allows for tuning the product gas for other applications (Dieterich et al., 2020).

The challenges of syngas production with SOEC include:

- High operating temperature: The process requires high temperatures (700–1000  $^{\circ}$ C) to achieve sufficient ionic conductivity and electrochemical activity. This poses thermal stress, material degradation, heat management, and safety (Dieterich et al., 2020).
- Long-term stability: The process suffers from degradation mechanisms such as electrode delamination, interfacial reactions, microstructural changes, and poisoning by impurities. These affect the performance and durability of the cells over time(Dieterich et al., 2020).
- Scale-up: The process faces technical difficulties in scaling from laboratory-scale cells to large-scale stacks and systems. These include cell design optimisation, gas distribution uniformity, thermal management, system integration, and cost reduction (Dieterich et al., 2020).

# 3.1.2. Indirect  $CO<sub>2</sub>$ -to-methanol via syngas intermediate

Indirect  $CO_2$ -to-methanol uses a hybrid  $CO_2/H_2O$  co-electrolysis approach combined with conventional methanol synthesis. The renewable syngas produced is converted to methanol via a coper-based catalyst, reaching a faradaic efficiency of 98%(Kylee et al., 2021) using syngas with an  $H<sub>2</sub>/CO$  ratio of 2:1 via the following overall reaction:

## $CO + 2H_2 \rightarrow CH_3OH(4)$

Acknowledging that  $CO<sub>2</sub>/H<sub>2</sub>O$  co-electrolysis is a nascent technology, syngas is usually obtained from biomass gasification.

### 3.2. Cost structure

<span id="page-27-0"></span>Zhang & Desideri, (2020) presents a techno-economic optimisation of a power-to-methanol (PtM) system with co-electrolysis of  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$  in solid-oxide electrolysers. The system converts renewable electricity to methanol by producing syngas from co-electrolysis of  $CO<sub>2</sub>$  and H2O, then converting the syngas to methanol. The system achieves a high energy efficiency of 72% but has a high methanol production cost of 471  $\epsilon$ /ton and payback time of over 11 years. The sensitivity analysis shows that reducing electricity price from 60 to 20  $\epsilon$ /MWh reduces methanol cost from 471 to 137.7  $\epsilon$ /ton.

There is limited research on the economic assessment of producing methanol by this pathway. Apart from Zhang & Desideri, (2020), no article has been found on the economic assessment of this pathways. Abad et al., (2021) discussed the technical feasibility but did not conduct an economic analysis. Andika et al., (2018) also examined technical feasibility without economic evaluation. The closest paper was Ferguson et al., (2021) who conducted a techno-economic feasibility study of producing methanol from using a mixture of Hydrogen produced by SOEC and CO from biomass gasification. The capital cost of the SOEC system (\$33 million) was identified as the major contributor, comprising 68% of the total capital costs. Ferguson et al., (2021) note that with a projected halving of SOEC costs by 2030, at interest rates below 4% the project is profitable with selling cost of 0.61  $\epsilon$ /kg. However, at current SOEC costs, the economics are not favourable for competitive methanol production through this method. Reductions in capital costs of SOECs and lower interest rates could improve feasibility in the future.

#### <span id="page-27-1"></span>4. Analytical Review on existing previous studies and research gap

Since the late 20th century, renewable methanol has gained attention due to its potential to reduce greenhouse gas emissions and provide a clean and versatile fuel for various applications.

The cost of e-methanol is largely influenced by the cost of hydrogen and  $CO<sub>2</sub>$ , according to the International Renewable Energy Agency, (2021). The agency estimated that e-methanol cost

ranges from 1200 to 2400 USD/t, with  $CO<sub>2</sub>$  capture cost of 300-600 USD/t. Bos et al., (2020) also found that the cost of methanol depends on the cost of electrolysis and  $CO<sub>2</sub>$  capture. They reported that the capital cost split-up of the plant were roughly 45% for the electrolysers, 50% for the  $CO<sub>2</sub>$  capture and 5% for the methanol section excluding the wind turbines. The study suggested that sorbent costs were the main component of the capital cost of  $CO<sub>2</sub>$  capture, accounting for 71.8% of it, and recommended further research on sorbent durability and capacity. The study also indicated that heat for adsorption-desorption was the major operational cost for  $CO<sub>2</sub>$  capture but did not specify how much. A report by the International Energy Agency, (2021) stated that heat represented 80% of the total energy required for  $CO<sub>2</sub>$  capture using solid sorbents. This could have a significant impact on the capture cost, as Fasihi et al., (2019) demonstrated in their techno-economic assessment of different CO<sub>2</sub> plants. They calculated a levelized cost of 133  $\epsilon$ /kg CO<sub>2</sub> and 222  $\epsilon$ /kg CO<sub>2</sub> for waste heat and without waste heat respectively.

Most of the studies on e-methanol agrees that the cost of e-methanol depends on hydrogen (Bos et al., 2020; Nizami et al., 2022; Schmidt et al., 2018; Sollai et al., 2023). The International Renewable Energy Agency, (2021) reported in its "Renewable Methanol: Outlook" that the cost of e-methanol would decline as the cost of renewable hydrogen decreased. Bhandari & Shah, (2021) examined the cost of hydrogen and found that it was largely influenced by the cost of electricity and the capital cost of electrolysers. This was corroborated by the International Energy Agency, (2022) in its Global Hydrogen Review, which projected that by 2030, hydrogen from solar PV could drop below USD 1.5/kg  $H_2$  and by 2050 below USD 1/kg  $H_2$  in regions with favourable solar conditions and consequently low electricity costs from solar PV, which accounted for approximately 55% of the total hydrogen production costs in these cases.

The same review from the International Renewable Energy Agency, (2021) suggests that an alternative and more efficient method for producing e-methanol involves co-electrolysis to generate CO and H2, followed by converting the syngas to e-methanol, although this approach is not as developed as conventional water electrolysis (conventional water electrolysis is in the megawatt range, while this co-electrolysis route is at the lab, kilowatt scale). The catalytic conversion of syngas to methanol is used in fossil-based methanol where the feedstock cost represent the major cost according to a review of power-to-liquid by Schmidt et al., (2018). The review also says that syngas conversion to methanol consume less feedstock than hydrogen to methanol. Kgwedi et al., (2023) share the same idea in their techno-economic assessment of methanol production from syngas from biomass gasification process where syngas to methanol need H<sub>2</sub>: CO input ratio of 2:1 while Ferguson et al., (2021) and Bos et al., (2020) give H<sub>2</sub>: CO<sub>2</sub>

input ratio of 3:1 for hydrogen to methanol process. For Ferguson et al., (2021), renewable syngas could be produced from solid oxide electrolysis Cell but the technology is in lab scale and not much data isn't available in the literature. Their study did not perform a co-electrolysis, instead they use hydrogen from solid oxide electrolysis Cell and mix it with CO from biomass to have syngas for methanol production. The economic assessment shows that the capital cost of SOEC represents more than 68% of the total investment. For Zhang & Desideri, (2020) in their optimization of power-to-methanol using co-electrolysis process, the levelized cost of methanol were 471  $\epsilon$ /ton with high energy efficiency. No other study has been found for comparison to their results proving that there are limited knowledge about the cost structure of methanol using syngas from co-electrolysis process.

If the economics of the full process of coupling co-electrolysis and methanol production could not be found, focusing on co-electrolysis to syngas by solid oxide electrolysis Cell could help to understand the cost structure of syngas. Unfortunately, there are still not much literature about the economics of this process compared to hydrogen production with SOEC. The technical feasibility is proven in some studies like (Ali et al., 2020; Dogu et al., 2019; Salomone et al., 2019) but only Jambur, (2022) has been found on the economics assessment of  $H_2O/CO_2$  coelectrolysis for syngas production with Solid Oxid Electrolysis Cell. The Levelized cost of syngas found by the study were 0.69  $\epsilon$ /kg and that cost is five times the cost of fossil-based syngas according to the study. The sensitivity analysis highlighted that electricity cost is the major cost followed by the capital expenditure of solid oxide electrolysis cell.

The economics of e-methanol using syngas via  $CO<sub>2</sub>/H<sub>2</sub>O$  electrolysis is not well studied and understood like for hydrogen and carbon capture. The combination of  $CO<sub>2</sub>$  capture and SOEC for co-electrolysis could offer a real cost improvement compared to hydrogen to methanol due to the high energy efficiency of SOEC and the feedstock ratio need for syngas conversion to methanol. Clearly only one study have been found on the economics of this process, but it did not use carbon capture for  $CO<sub>2</sub>$  source. A clear understanding of the cost structure of this process represent the gap in the literature that our study is willing to fill. Our study will compare the two production pathways and analyse the cost structure, find the cost drivers, and identify area of improvement.

### <span id="page-30-0"></span>5. Methanol value chain

According to Jarvis & Samsatli, (2018), a value chain is a network of technologies and infrastructures (such as conversion, transportation, and storage) along with its associated activities (such as sourcing raw materials, processing, logistics, inventory management, waste management) required to convert low-value resources to high-value products and energy services and deliver them to customers. As the product moves from one player in the chain to another, it is assumed to gain value. E-methanol value chain involves the production of raw materials (involving  $CO<sub>2</sub>$  capture and hydrogen or Syngas production), technologies that convert the feedstocks into valuable products, sourcing of the type of energy used to drive all of the transformation processes required to convert feedstocks to e-methanol, transport of energy and materials to where they are needed, and delivering the products to customers, all in order to create value (economic, environmental, social etc.).

# Chapter III: Materials and Methods

<span id="page-31-0"></span>The methodology of this research is structured to address properly the research questions. Secondary data from the literature are used and processed using Microsoft Excel to design an emethanol plant and to find the inputs and outputs for the first and second research questions. The levelized cost method is used as the economic approach for addressing the third research question based on Nizami et al., (2022). The levelized cost of each input and output are calculated and the cost drivers of e-methanol production are identified and analysed using a sensitivity analysis with What-if scenario in Microsoft Excel. The value added at each stage of the process is investigated by the fourth research question. The main steps are Data collection, Process design and modelling, Levelized cost calculation, Sensitivity analysis and Analysis of value added at each stage or production.

#### <span id="page-31-1"></span>1. Data collection

Data collection is an in-depth result of the literature review. Due to time constraints and the unavailability of primary data, secondary data were used from the literature. The databases used are science-direct, pubs.rsc., IRENA (International Renewable Energy Agency), IEA (International Energy Agency), researchgate.net, NASA power access viewer and Global Solar Atlas. The data used for this work will be provided later in the Process Design and Economic Evaluation section.

### <span id="page-31-2"></span>2. System configuration and Modelling

Two scenarios are studied in this research. The first scenario is called the SOEC scenario because it uses a solid oxide electrolysis cell (SOEC) while the second scenario is called the PEM scenario due to the use of a Proton Exchange Membrane (PEM) electrolyser. The specific description is as follows:

Scenario 1: The PV array is used to generate and store renewable energy for the needs of the entire system. Solid sorbent direct air capture (S-DAC) provides co-adsorption/desorption of  $H<sub>2</sub>O$  and  $CO<sub>2</sub>$  to feed a solid oxide electrolysis cell to produce syngas through  $CO<sub>2</sub>/H<sub>2</sub>O$  coelectrolysis. The syngas is then converted to methanol by the conventional process known as CO hydrogenation or indirect  $CO<sub>2</sub>$  hydrogenation in the methanol synthesiser.

Scenario 2: With PV and battery as the power source and solid sorbent direct air capture (S-DAC) for CO<sub>2</sub>/H<sub>2</sub>O co-adsorption, a proton exchange membrane (PEM) is used to produce hydrogen. The  $H_2$  as well as the captured  $CO_2$  are then routed to a methanol synthesiser to produce methanol through the process known as direct  $CO<sub>2</sub>$  hydrogenation.

### <span id="page-32-0"></span>2.1. Assumption

The assumptions applied in this study are vital for providing a structured approach to the complex problem of renewable methanol production. The key assumptions made are as follows:

- An annual methanol production target of 50,000 tons is assumed for both scenarios.
- The plant is designed to operate 20 hours a day, leading to a total operational time of 7,300 hours per year.
- The project lifetime is projected to be 25 years, which is based on the expected lifespan of key components such as the PV system, DAC, and methanol reactor.
- The electrolysers are designed to operate at an 80% load.
- The sorbent used for DAC, Lewatit VP OC 1065, has a co-adsorption capacity based on the range of temperature and relative humidity as determined by Martínez, (2020)
- For DAC, it is assumed that the system uses electrical energy and waste heat for desorption.
- The location for the PV system and DAC is assumed to be Tengrela, Cote d'Ivoire, with climate data obtained from NASA's solar power data access viewer.

# <span id="page-32-1"></span>2.2. Process Design of methanol reactor

The design of the methanol reactor is crucial to our study. The reactor is responsible for the conversion of carbon dioxide and hydrogen or syngas into methanol, a key step in the overall process. For both scenarios, the process and reactions are different since the inputs are different. Scenario 1 is called CO hydrogenation or indirect  $CO<sub>2</sub>$  hydrogenation. For the second scenario, it is called direct hydrogenation of CO2. Parameters used for the determination of inputs and outputs are summarized in the [Table 3](#page-33-0) below.

<span id="page-33-0"></span>

Table 3: Data for Methanol synthesis

#### - Mass flow rate

The mass flow rate is essential for cost estimation. The equilibrium reaction of both scenarios is used. The first scenario involves direct CO hydrogenation or indirect  $CO<sub>2</sub>$  hydrogenation with CO and  $H_2$  as feedstock with a feeding ratio of  $H_2$ /CO=2 (Ban et al., 2020).

#### $CO + 2H_2 \rightarrow CH_3OH$  (5)

The second scenario involves direct  $CO<sub>2</sub>$  hydrogenation with  $CO<sub>2</sub>$  and  $H<sub>2</sub>$  as feedstock with a feeding ratio of  $H_2/CO_2 = 3$  (Elnabawy et al., 2020).

$$
CO_2 + 3H_2 \longrightarrow CH_3OH + H_2O \quad (6)
$$

The empirical formula to determine inputs reactants and products from working reaction is used for both scenarios and the efficiency of the reactor is applied.

From equation 1, every mol of  $CO<sub>2</sub>$  corresponds to 1 mol of MeOH.

$$
mCO_2 = \left(\frac{MCO_2 \times mCH_3OH}{MCH_3OH}\right)/n
$$
 (7)

Where:

 $mCO<sub>2</sub>$  and  $mCH<sub>3</sub>COH$  are the mass of  $CO<sub>2</sub>$  and  $CH<sub>3</sub>COH$  respectively

MCO<sup>2</sup> and MCH3OH are the molecular mass of CO<sup>2</sup> and CH3OH

n is the efficiency of the reactor

From the same equation, 3mol of  $H_2$  give 1mol of methanol, which leads to the following formula.

$$
mH_2 = \left(\frac{MH_2 \times mCH_3OH}{3MCH_3OH}\right)/n \quad (8)
$$

Where:

 $mH_2$  and mCH<sub>3</sub>COH are the mass of  $H_2$  and CH<sub>3</sub>COH, respectively.

 $MH<sub>2</sub>$  and MCH<sub>3</sub>OH are the molecular mass of H<sub>2</sub> and CH3OH

N is the efficiency of the reactor

The reactor design is based on the Fisher-Tropsch reactor, and its efficiency is applied to the reaction. The input rates required to produce 1 kg of methanol are determined and scaled based on the desired capacity and working time to find the feeding rate.

- Energy balance

The energy balance is crucial for  $CO<sub>2</sub>$  to methanol conversion since the reactions are exothermic and generate heat. However, for the scope of this study, focus is not on heat recuperation and integration. Only the electrical energy is considered, obtained from literature, and applied to our production. The energy consumption for 1 kg of MeOH production is simply multiplied by the production rate found earlier.

### <span id="page-34-0"></span>2.3. Process Design of Electrolysers

Two types of electrolysers are used in our study: the Solid Oxide Electrolysis Cell (SOEC) for syngas production in the first scenario and the Proton Exchange Membrane (PEM) electrolyser for hydrogen production in the second scenario.

### 2.3.1. Solid Oxide Electrolysis Cell

The Sunfire SYNLINK electrolyser with a 2.89 MW unit capacity is used for Scenario 1. It is the only SOEC electrolyser with an available online factsheet that can produce syngas with a 2:1 ratio. The factsheet's technical data is used to determine the  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$  input per hour and the energy per hour based on the syngas input required for CO hydrogenation. In this case, there is no need to use the heating value of  $H_2$  and efficiency of SOEC to determine the inputs and outputs rate. Since Sunfire Synlink is commercial, it provides accurate data, so no need to rely on experimental lab scale data. However, the stack lifetime was not provided in the factsheet. It has been completed from the literature. [Table 4](#page-35-0) below presents the data.

<span id="page-35-0"></span>



- Mass flow rate

The production rate provided in the factsheet is volume per hour. The density of syngas with ratio 2 is used to convert this unit in mass per hour (kg/h). An assumption of 80% load is used. The syngas input per hour for MeOH reactor represents the desired output for input determination.

- Energy flow rate

The energy requirement from the factsheet is simply converted to KWh/kg and multiply by the desired output per hour.

# 2.3.2. Proton Exchange Membrane

H-TEC electrolyser with a 10 MW unit capacity is selected for Scenario 2. The PEM electrolyser is a well-developed technology, and the literature provides information on operating hours and H-TEC is chosen because it has lower water consumption per kg of  $H_2$  produced.

<span id="page-36-0"></span>

#### Table 5: Parameters for Proton Exchange Membrane

- Mass and energy flow

The same procedure regarding the load capacity has been used in the case of PEM. The desired output here is simply the hourly hydrogen demand of the MeOH reactor.

- <span id="page-36-1"></span>2.4. Process Design of Direct Air Capture (DAC)
- Choice of the type of DAC

The overall design depends mainly on the chosen Direct Air Capture (DAC) technology. This study selects temperature swing adsorption solid Direct Air Capture (TSA-DAC) as the DAC type. This DAC type uses amine-based sorbents such as Lewatit VP OC 1065 and works at ambient temperature.

- Choice of sorbent

The sorbent is a key component of solid DAC as it enables the co-adsorption and desorption of CO<sup>2</sup> and H2O. Previous studies have demonstrated the co-adsorption capacity of Zeolite and Lewatit VP OC 1065 sorbents at various temperatures and relative humidity levels.



<span id="page-37-1"></span>Figure 3: Molar water captured as a function of relative humidity for the sorbent Lewatit VP OC 1065

#### Source: (Martínez, 2020)

This graph shows that there is no big change in temperature ranges from 15℃ to 35℃. However, for every change in relative humidity, a change in  $H_2O$  capture is observed. The relative humidity of the community selected and the average temperature are assessed to find the H2O corresponding capture using this graph.

- Climate data

It consists mainly of temperature and relative humidity. Hourly relative humidity and temperature have been collected from NASA data access viewer. The average, lowest and highest values has been calculated for each parameter and the average value is used for the design while the low and highest values are used in sensitivity analysis for worse and best-case scenarios.

<span id="page-37-0"></span>

Location: Korhogo	Lowest	Average	Highest
Temperature °C	15.08	26.24	38.8
Relative humidity %	10.06	70.74	100

Table 6: Climate data used for Solid Direct Air Capture

### Mass flow

Relative humidity of 70% as well as average temperature of 25℃ is used on the [Figure 3](#page-37-1) and corresponding  $H_2O$  capture in mmol of  $H_2O$  per kg of sorbent is found. Also, the  $CO_2$  capture from the same literature is used. The amount of  $CO<sub>2</sub>$  needed per hour for both scenarios is divided by the capture rate to find the amount of sorbent for each scenario.

- Energy flow

Solid TSA DAC has the advantage of using electrical energy for some components, mainly fans, and waste heat for desorption. According to IEA (2022), heat accounts for 75-80% of energy demand. Waste heat from industry or heat from the methanol reactor could help significantly reduce the cost of energy. However, this study does not include heat integration. Therefore, electricity demand is considered as reported in the literature, and waste heat from industry is assumed.

All the data used for the process design of DAC is summarised in [Table 7](#page-38-0) below:

<span id="page-38-0"></span>

	Values	Units	Sources
Technology	Solid Direct Air Capture		
Type of DAC	Temperature swing adsorption		(Wiegner et al.,
	(TSA) adsorption/desorption		2022
Sorbent	amine functionalised Lewatit VP OC		Martínez, (2020)
	1065		
Sorbent	1 year	year	(Panda et al., 2023)
Lifetime			
Adsorption	25-90 $\degree$ C	$\rm ^{\circ}C$	(Wiegner et al.,
temperature			2022
Water capture	7.5 for RH 70%	mol/kg	(Martínez, 2020;
			Young et al., 2021)
$CO2$ capture	$2.5 \text{ mol/kg}$	mol/kg	(Martínez, 2020)
Energy	250	$kwh_{el}/tCO2$	(Fasihi et al., 2019)
electrical energy			
Thermal energy	1150		$kwh_{th}/tCO_2$ (Panda et al., 2023)

Table 7: Data for solid Direct Air Capture

### <span id="page-39-0"></span>2.5. Sizing of the PV system

- PV panels

To obtain the climate data for renewable PV design and Direct Air Capture design, a specific site needs to be chosen. Therefore, the case study site selected for this study is at Tengrela (Latitude: 8.5078 and Longitude: -5.8339) in Cote d'Ivoire since Cote d'Ivoire is the base location of the project. The climate data is obtained from NASA solar power data access viewer. This source provides the daily average irradiance, as well as the hourly irradiance, relative humidity, and temperature for this location throughout the year 2021. The design started with data for 2022 but there was an error, which is what lead to the choice of 2021.

The equation [\(9\)](#page-39-1) below from Bhandari  $\&$  Shah, (2021) is used to calculate the required PV system size.

<span id="page-39-1"></span>
$$
Ppeak (KW) = \frac{E_d(KWh) \times I_{stc}(KW/m^2)}{G(\frac{KWh}{m^2}) \times Q} \hspace{2mm} (9)
$$

Ppeak: the Required solar PV capacity in kW

Ed: Energy demand in kWh per day.

Istc: Radiation at standard test condition in kW/m2 (value 1 kW/ m2)

G: Global solar radiation in kWh/m2 /day.

Q: Quality factor or performance ratio

From this Ppeak value, the energy generation from this system is calculated for every hour in the year. The energy generated is calculated using equation [\(10\)](#page-39-2) below.

<span id="page-39-2"></span>
$$
E_{gen}(KWh) = \frac{P_{peak}(KW) \times G(\frac{KWh}{m^2}) \times Q}{I_{stc}(\frac{KW}{m^2})}
$$
 (10)

Where Egen is the Energy generated

### - Sizing of the battery

For off grid systems, the battery size is calculated using the equation [\(11\)](#page-40-0) below.

<span id="page-40-0"></span>**Battery size**  $(KWh) = \frac{Ed(KWh)*Day\ of\ automorphism}{DQD\times m}$  $\frac{\partial^* Day \, dy \, dy \, du \, \omega}{\partial \omega \times n_{sys}}$  (11)

where Ed – is the daily demand.

DOD – depth of discharge of the battery

Day of autonomy

Nsys is the overall battery system efficiency.

According to (Bhandari & Shah, 2021), Equation [\(12\)](#page-40-1) is the general equation used to do battery sizing. Using this equation often leads to large battery sizes. So, in order to optimize the battery size, the author proposed the equation below.

<span id="page-40-1"></span>
$$
Battery \, size = \frac{E_{req}(KWh)}{DOD \times n_{sys}} \quad (12)
$$

Where Ereq is the Energy to be supplied from the battery

- Battery size verification

To validate the battery capacity, the hourly energy generation and battery charging/discharging cycles were modelled.

When the PV system generates surplus energy and the battery is not fully charged, the excess is stored in the battery (charging). When the PV system cannot meet the energy demand, the deficit is supplied by discharging the battery. To analyse the charging and discharging over 8,760 hours, an equation was implemented in Excel. If there is stored energy in the battery during Hour 1 and a surplus in Hour 2, the battery will charge and store the excess. The sum of the energy eHour 1 and eHour 2 will equal the new battery energy for Hour 2. If this sum exceeds battery capacity, no additional energy can be stored, and eHour 2 will equal the battery size. For subsequent hours like Hour 2 and Hour 3, if there is a deficit in Hour 3, energy will discharge from the battery and eHour 3 will be less than eHour 2. The hourly energy values were evaluated for the full year. If all values are positive, the battery can store the excess and meet any shortfalls.

> *Charging/discharging* "Hour2" = *if* [sum (EHour1, EHour2)  $\geq$  batery size, batery size, sum (EHour1, EHour2)

Here 'eHour1', 'eHour2' and 'Hour2' mean the amount of energy in the battery on hour 1, amount of energy in the battery on hour 2 and either the surplus or the deficit of hour 2.

### <span id="page-41-1"></span>3. Economic assessment

Most of the technologies involved in e-methanol production are still in the early stages. Only PV has an attaint maturity level. High-temperature co-electrolysis is still under development and large demonstration units for long-term operation do not exist currently. Even though liquid DAC is a well-known technology, solid DAC is still in its early stages and very few studies have been conducted on the co-adsorption of  $CO<sub>2</sub>/H<sub>2</sub>O$  under different climate data. Accurate cost assessment is challenging due to several uncertainties related to the technologies, such as estimating manufacturing cost, lifetime, and reliability in different working conditions. The parameters used in the economic assessment in this thesis were based on few studies available.

<span id="page-41-0"></span>

Technology	<b>CAPEX</b>	<b>OPEX</b>	Lifetime	Source
PV monocrystalline	539.4	1%	25	(Bhandari & Shah, 2021;
	E/KW			Nizami et al., 2022)
Lithium-ion battery	179.8	0.027	15	(Bhandari & Shah, 2021;
	E/KWh	E/KWh		Nizami et al., 2022)
Direct Air Capture	$79.11 -$	4%	25	(Wu et al., 2022)
(DAC)	204.97			
	$\epsilon$ /tCO <sub>2</sub>			
Sorbent cost	$30 \text{ E/kg}$		$\mathbf{1}$	(Bos et al., 2020b)
Solid Oxide	2000 €/KW	2%	25	(Hauch et al., 2020)
Electrolysis Cell				
(SOEC)				
Stack replacement	$450 \text{ E/KW}$		48000h	(Jambur, 2022)
Proton Exchange	1000 €/KW	1.32%	25	(Bhandari & Shah, 2021)
Membrane (PEM)				
Stack replacement	350		60000h	(Bhandari & Shah,
				2021) (International Energy
				Agency., 2022)
<b>Methanol Reactor</b>	661.74/t	2%	25	(Nizami et al., 2022)
(MeOH)	MeOH			
Catalyst cost	15 €/ $kg$		$\overline{4}$	(Bos et al., 2020b)

Table 8: Cost components for economics assessment

PV cost has been found in dollars 2020 and has been converted to euro 2020 using the average 2020 exchange rate of 0.877€ found on (*Yearly Average Currency Exchange Rates | Internal Revenue Service*, n.d.)

To successfully model the cost structure, the methodology used consist primarily of cost components identification. Cost components like Capital cost, operating fixed and variable costs have been identified in previous studies. Levelized costs have been used to model the cost structure and cost drivers have been identified to perform a sensitivity analysis.

### <span id="page-42-0"></span>3.1. Levelized cost of electricity (LCOE)

Levelized Cost of Electricity (LCOE) is an economic measure used to compare the lifetime costs of generating electricity across various generation technologies. It can be expressed by the equation [\(13\)](#page-42-1) below:

<span id="page-42-1"></span>
$$
LCOE = \frac{I + \sum_{t=1}^{25} \frac{A_t}{(1+r)^t}}{\sum_{t=1}^{8760} \frac{Gen_t}{(1+r)^t}}
$$
(13)

Where I is the upfront investment (capital expenditure)

At is the annual total operational expenditure time the lifetime

Gen is the annual generation time the lifetime

R is the discount rate 5% according to (Szabó et al., 2021)

The lifetime costs for generation can be categorized into the following groups:

Capital Costs: up-front costs to construct a power plant.

Operation and Maintenance annual (O&M) Costs: costs incurred to run a power plant. These costs can be sub-categorized into fixed and variable costs. Fixed O&M costs are incurred regardless of the plant generating electricity; they are comprised of personnel salaries, security costs, insurance, etc. Variable O&M costs are directly linked to the generation of the power.

The Annual operation cost can be rewriting as follow in equation [\(14\):](#page-42-2)

<span id="page-42-2"></span>
$$
At = (Opex_{fixed} + Opex_{variable}) \times t \quad (14)
$$

with Opex<sub>fixed</sub> the fixed cost and Opex<sub>variable</sub> the variable cost or fuel cost. For PV system, fuel cost is considered to zero.

# <span id="page-43-0"></span>3.2. Levelized cost of  $CO<sub>2</sub>$  and Water (LCOD and LCOW)

The levelised cost of  $CO_2$  and  $H_2O$  represent the cost of capture in our study. The lifetime costs are split 50% each between  $CO_2$  and  $H_2O$  for this purpose. The LCOD is corresponded by 50% of the lifetime cost divided by the  $CO<sub>2</sub>$  lifetime output. The same is done to find the LCOW. The reason for this share is that water is a desired output in our case since it is a main input for the electrolysers. The calculation of the LCOW is therefore important to determine the contribution of the water captured by the DAC to the overall cost structure of the final product. Equatio[n \(15\)](#page-43-2) and [\(17\)](#page-43-3) are used for LCOD and LCOW respectively:

<span id="page-43-2"></span>
$$
LCDD = \frac{50\% \times (I + \sum_{t=1}^{25} \frac{A_t}{(1+r)^t})}{\sum_{t=1}^{25} \frac{CO2_t}{(1+r)^t}} (15) \quad \text{and} \quad LCOW = \frac{50\% \times (I + \sum_{t=1}^{25} \frac{A_t}{(1+r)^t})}{\sum_{t=1}^{25} \frac{H2O_t}{(1+r)^t}} (16)
$$

Where  $CO_{2t}$  and H<sub>2</sub>Ot are the lifecycle output of  $CO_2$  and H<sub>2</sub>O respectively.

According to Fasihi et al., (2019) the variable cost for DAC using waste heat is expressed using equation [\(17\)](#page-43-3) below:

<span id="page-43-3"></span>
$$
Opex_{variable} = DAc_{el.input} \times LCOE
$$
 (17)

With equation ([17](#page-43-3), the annual total operating cost of capture can be expressed using equation [\(18\)](#page-43-4) below:

<span id="page-43-5"></span><span id="page-43-4"></span><span id="page-43-1"></span>
$$
At_D = Oper_{fixed} + DAC_{el.input} \times LCOE
$$
 (18)

### 3.3. Levelized cost of Hydrogen and syngas (LCOH and LCOS)

The levelized cost of Hydrogen is determined by equation [\(13\)](#page-42-1) with the annual total operating cost expressed by the equation [\(19\)](#page-43-5) below since electricity and water are the inputs fuel.

$$
At_h = (Oper_{fixed} + PEM_{el.input} \times LCOE + PEM_{H2O.input} \times LCOW) \times t
$$
 (19)

Similarly, as the inputs feedstocks for syngas are electricity,  $H_2O$  and  $CO_2$ , the annual total cost for levelized cost of syngas determination is expressed in equation [\(20\)](#page-44-2) :

 $At_s = (0 p e x_{fixed} + S O E C_{el. input} \times L C O E + S O E C_{H2O. input} \times L C O W + S O E C_{CO2. input} \times$  $L(COD) \times t$  (20)

### <span id="page-44-2"></span><span id="page-44-0"></span>3.4. Levelized cost of methanol (LCOM)

The levelized cost of methanol is also expressed using equation [\(13\).](#page-42-1) The annual operating expenses for scenario 1 consider fixed costs, syngas cost and  $CO<sub>2</sub>$  cost along with electricity cost.

# $At_{m1} = Oper_{fixed} + reactor_{el.input} \times LCOE + reactor_{syngas.input} \times LCOW +$  $reactor_{CO2, input} \times LGOD$  (21)

Similarly for the scenario 2, the inputs identified are  $CO<sub>2</sub>$  cost and Hydrogen cost along with electricity cost.

# $At_{m2} = \textit{Oper}_{fixed} + \textit{reactor}_{el.input} \times \textit{LCOE} + \textit{reactor}_{H20.input} \times \textit{LCOW} +$  $reactor_{CO2, input} \times LCD$  (22)

### <span id="page-44-1"></span>4. Sensitivity Analysis

Sensitivity analysis is a crucial aspect of economic evaluation, aimed at understanding the effects of altering an independent variable (input) on a dependent variable (target) under predefined assumptions. In our study, "what-if" analysis feature were employed in Excel's toolbox to conduct this evaluation. The variables considered in the sensitivity analysis are based on their potential impacts on the cost structure. Specifically, the following important factors have been the area of interest and their choice is explained below:

- Electricity cost: This is the main determinant of hydrogen and syngas costs, which are the major inputs identified for methanol production. Electricity cost depends on the photovoltaic system configuration and performance and the use of not of battery. The future cost of battery found in Mauler et al., (2021) has been used to show how battery cost affects the electricity cost and LCOM.
- **Capital expenditure of direct air capture**: This is the cost of acquisition and installing the direct air capture system using solid sorbents. Direct air capture is still in early stages and the cost is expected to decrease in the next decades. The standard learning curve

approach is applied for estimating the DAC capex development, according to Fasihi et al., (2019) with the equation ([23](#page-45-0) [below:](#page-45-1)

*Capex<sub>new</sub>* = *Capex<sub>initial</sub>* 
$$
\frac{Production_{new}}{Production_{initial}}
$$
  $)$ <sup>-b</sup> (23)

<span id="page-45-1"></span>The abbreviations are as follows: capital expenditure, capex, progress ratio, PR, binary exponential expression of the progress ratio, b, learning rate, LR, applied to cumulative historical production for specific years:

<span id="page-45-0"></span>
$$
PR = (2)^{-b} \quad (24)
$$
  

$$
LR = 1 - PR \quad (25)
$$

For an estimate of the future cost of DAC according to the formulas used, three inputs are necessary: (1) The initial capex is taken from [Table 8;](#page-41-0) (2) Cumulative historical demand for DAC capacity is taken from (Fasihi et al., 2019) and (3) DAC system learning rate is taken from (Fasihi et al., 2019).

- **Capital expenditure and stack cost of SOEC**: Solid Oxide Electrolysis Cell is an emerging technology that has high capital cost, high stack cost and low lifetime compared to other electrolysis technologies. Stack cost and capital expenditure prediction found in literature for 2050 has been used to show how they affect the syngas cost and LCOM.
- **Relative humidity**: This is an environmental factor that affects the sorbent's capture capacity and regeneration rate. Relative humidity varies depending on the location and climate conditions. The database of NASA data access viewer has been used to obtain the annual variability of relative humidity in the chosen region. The lowest and highest relative humidity are used as the worst and best climate cases, respectively, to show how they affect the capture cost and LCOM.

Chapter IV: Results and Discussion

- <span id="page-46-2"></span><span id="page-46-1"></span>1. Technical parameters
- <span id="page-46-3"></span>1.1. Input and outputs identification for the first scenario



Figure 4: Flow chart with inputs and outputs scenario 1

<span id="page-46-0"></span>This [Figure 4](#page-46-0) shows methanol production in scenario 1 using the SOEC cell for syngas. It gives details of hourly production, inputs, and outputs with precise hourly quantities, as well as the capacity of the technologies used. As the operation of scenario 1 has already been discussed earlier in the methodology section, it will not be explained in detail here. However, the detail that attracts attention here is the production of water by the DAC. In fact, the water production is far greater than the water requirements for co-electrolysis. This excess water can be sold and have an added value to the production cost structure.



<span id="page-47-2"></span>1.2. Input and outputs identification for the second scenario

Figure 5: Flow chart with inputs and outputs scenario 2

<span id="page-47-1"></span>Exactly like the previous flow chart, the one presented in Figure 5 shows us the details of methanol production in scenario 2 using the hydrogen produced by the PEM Cell. The hourly production of each technology, their capacities and the inputs and outputs are marked. Note that unlike scenario 1, the output obtained here is  $CO<sub>2</sub>$ . This excess  $CO<sub>2</sub>$  can be sold to local or international companies.

<span id="page-47-3"></span>2. Levelized cost of production.

In the [Table 9,](#page-47-0) show the levelized costs of different energy products and processes based on our assumptions and scenarios. The main findings are compared to the literature.

<span id="page-47-0"></span>

Parameters   Unit		Scenario1:	Scenario <sub>2</sub> :	Literature
		<b>SOEC</b>	<b>PEM</b>	
<b>LCOE</b>	E/KWh	0.07	0.07	0.11 $\epsilon$ /kWh (Nizami et al.,
				(2022)
<b>LCOD</b>	$\epsilon$ /kg CO <sub>2</sub>	0.08	0.08	0.133 €/kg (Fasihi et al., 2019)
<b>LCOW</b>	$E/kgH_2O$	0.07	0.07	

Table 9: Levelized cost for each technology.



LCOE for PV system with battery has usually bigger cost than PV system without battery. Our LCOE for both scenarios are  $\epsilon$  0.07 per kWh. In the study of Nizami et al., (2022), LCOE for PV with battery is  $\epsilon$ 0.125 per kWh in Indonesia. According to Kost et al., (2021) LCOE for PV with battery ranges from  $0.08 \text{ E/KWh}$  to  $0.20 \text{ E/KWh}$ .

The Levelized cost of  $CO<sub>2</sub>$  (LCOD) and the Levelized cost of H<sub>2</sub>O (LCOW) represent the levelized cost of capture. Assuming using waste heat, the levelized cost of  $CO<sub>2</sub>$  and the levelized cost of H<sub>2</sub>O are 0.08  $\epsilon$ /kg and 0.074  $\epsilon$ /kg respectively. This is predictable since the total cost is shared equally to calculate the LCOD and LCOW and the gaps between both outputs in kg is not considerable (0.91 kg  $CO_2$  per kgH<sub>2</sub>O). However, this is purely based on our climate conditions and the co-adsorption capacity of the sorbent. Changes in the climate conditions will change the outputs and consequently change the levelized cost of  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$ . In the literature, such method is not found. Only the levelized cost of  $CO<sub>2</sub>$  is assessed in all the literature found in the field even if  $H_2O$  is co-captured along with  $CO<sub>2</sub>$ . For example, Fasihi et al., (2019) have performed a Techno-economic assessment of CO<sup>2</sup> for Liquid and Solid direct air capture. He found a levelized cost of capture of 0.133€/kg assuming using waste heat for solid sorbent direct air capture. H<sub>2</sub>O captured were not considered in the economic assessment. For Sinha et al., (2017), different solid sorbent have been used for  $CO<sub>2</sub>-H<sub>2</sub>O$  co-adsorption and the levelized cost of capture ranges between 65  $\epsilon$ /tCO<sub>2</sub> to 122  $\epsilon$ /tCO<sub>2</sub>.

Levelized cost of hydrogen has been widely studied since hydrogen became one of the promising alternatives for fossil fuel. From Bhandari & Shah, (2021). LCOH ranges from 5 to 7 euros/kgH2. In the Global Hydrogen Review 2022 of the International Energy Agency, (2022), Levelized cost of hydrogen from solar and water electrolysis ranges from 4 to 8.5 USD/kg.

Co-electrolysis from SOEC is not well studied and most of the levelized cost of syngas found in literature are from natural gas processing or biomass gasification. Jambur, (2022) found a LCOS of 0.697  $\epsilon$ /kg using SOEC. As comparison to the fossil-based Syngas produced from natural gas

steam methane reforming, he found that co-electrolysis has a LCOS many times higher than the fossil-based Syngas which is 0.19  $\epsilon$ /kg.

Nizami et al., (2022) have found a LCOM of 1.464  $\epsilon$ /kg for PV-battery using PEM electrolyser with LCOE of 11 cent /KWh. Zhang & Desideri, (2020) have performed the techno-economic optimization of methanol production from syngas using SOEC. They were able to find a LCOM of  $0.471 \text{ E/kg}$ .

### <span id="page-49-0"></span>3. Cost structure and cost drivers' identification

Once the Levelized cost of each process has been determined, the major cost drivers in each step are identified by decomposing the Levelized cost. This allows for a transparent cost structure of each process to be outlined, and the contribution of each cost component within the system they participate in to be showcased.

### <span id="page-49-1"></span>3.1. Cost structure and cost drivers' identification for Methanol production

The initiation of cost driver identification was undertaken with the methanol reactor. The cost constituents encapsulated Capital Expenditure (CAPEX), fixed operational and maintenance expenses, labelled as OPEX\_fixed, along with variable operational costs.

In the context of the first scenario, the variable OPEX was dissected into individual expenses related to electricity, CO2, and syngas. Conversely, for scenario 2, the variable OPEX was categorised into costs of electricity, hydrogen, and CO2.

Each of these cost components was then evaluated for their respective contribution to the levelized cost. The findings of this analysis have been visually represented in the subsequent graph.



#### Figure 6: LCOM breakdown

<span id="page-50-0"></span>[Figure 6](#page-50-0) provides a clear indication that the major cost components are syngas and hydrogen costs in scenario 1 and scenario 2 respectively. Both these elements constitute over 90% of the Levelized Cost of Methanol (LCOM) in their respective scenarios. These findings align with those present in the current literature.

[Figure 6](#page-50-0) shows the cost breakdown of methanol production for the two scenarios. The main cost drivers in both scenarios are the feedstock costs, namely syngas and hydrogen, which account for more than 90% of the LCOM. This is consistent with the literature, which indicates that the cost of methanol is highly dependent on the cost and availability of syngas and hydrogen. For example, Nizami et al., (2022) reported that hydrogen production cost was the dominant factor in the LCOM of methanol synthesis using PV-battery and PEM electrolysis, while Kgwedi et al., (2023) and Kylee et al., (2021) found that syngas cost was the major contributor to the LCOM of methanol synthesis using different sources of syngas. Therefore, reducing the feedstock costs is crucial for improving the economic feasibility of methanol production.

# <span id="page-50-1"></span>3.2. Cost structure and cost drivers' identification for Syngas and hydrogen production

From the cost structure of the methanol reactor, it has been found that syngas cost and hydrogen cost are the major cost components for scenario 1 and scenario 2 respectively. A cost breakdown for both syngas production and hydrogen production are needed. To do so, the capital expenditure, stack replacement, operational fixed expenditure, and variable operation

expenditure have been considered. The variable operational expenditure consists of fuel costs like CO<sub>2</sub> cost, H<sub>2</sub>O cost, and electricity costs for syngas production in scenario 1. In scenario 2 the variable operational expenditure consists of fuel costs like electricity in  $H_2O$  cost.



Figure 7: LCOS and LCOH breakdown

<span id="page-51-0"></span>[Figure 7](#page-51-0) shows the breakdown of levelized cost of syngas (LCOS) and hydrogen (LCOH) production for the two scenarios of co-electrolysis and PEM electrolysis, respectively. The LCOS and LCOH are composed of four main components: electricity cost, capital expenditure, stack replacement cost, and operation and maintenance cost. The figure reveals that electricity cost is the dominant factor for both scenarios, accounting for 54% of LCOS and 70% of LCOH. It can be deducted that both co-electrolysis and PEM electrolysis are highly dependent on the electricity price and consumption. However, co-electrolysis has a lower electricity cost per unit of syngas than PEM electrolysis has per unit of hydrogen, due to its higher efficiency and lower energy requirement. This is consistent with the findings of Jambur (2022), who analysed the levelized cost of syngas production from SOEC and concluded that electricity is the major cost driver. Same findings for Bhandari & Shah, (2021) who performed a techno-economic analysis of hydrogen production using PEM electrolyser and found that electricity has the biggest share in the levelized cost of hydrogen.

The second largest component of LCOS and LCOH is capital expenditure, which includes the costs of the electrolyser, and balance of plant. Capital expenditure represents 14% of LCOS and 9% of LCOH. The higher capital expenditure for co-electrolysis than for PEM electrolysis is mainly due to the higher cost of the co-electrolyser, which requires more advanced materials and technologies. Stack replacement cost is another significant component of LCOS and LCOH, accounting for 14% and 9%, respectively. The stack costs are strongly dependent on the capital expenditure and stack replacement depends on the lifetime and degradation rate of the electrolyser stack, which are influenced by various factors such as operating conditions, material properties, and cell design. Initial expenditure together with stack replacement cost account for more than ¼ of the levelized cost of syngas with an exact share of 26% in our scenario.

The figure also shows that co-electrolysis has a lower LCOS has lower energy consumption than LCOH, indicating that co-electrolysis is more economically feasible than PEM electrolysis for producing syngas and hydrogen from renewable sources. However, both scenarios have a high LCOS and LCOH compared to the current market prices of syngas and hydrogen, which implies that further cost reductions are needed to make co-electrolysis and PEM electrolysis competitive with conventional methods. Therefore, reducing electricity cost, capital expenditure, and stack replacement cost is essential for improving the economic viability of co-electrolysis and PEM electrolysis.

# <span id="page-52-0"></span>3.3. Cost structure for Direct Air Capture

The cost structure of DAC system is composed of equipment costs or capex, sorbent costs, operational and maintenance fixed costs as well as operational variable costs. Here the sorbent cost is not included in the capex to evaluate its effects on the cost structure. The variable operational expenditure here is comprised of fuel costs like electricity. Th[e Figure 8](#page-53-0) below shows the effects of different cost components on the overall cost structure of the direct air capture system.



Figure 8: LCOD and LCOW breakdown

<span id="page-53-0"></span>[Figure 8](#page-53-0) shows the levelized cost of  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$  (LCOD and LCOH) production for the direct air capture (DAC) process using solid sorbents. The figure indicates that sorbent cost is the most significant factor for the levelized costs, accounting for 63% of the total cost. This is because the sorbent material is consumed during the DAC process and needs to be replaced periodically. Therefore, improving the sorbent performance and durability is essential for reducing the levelized costs. This agrees with the literature, which shows that sorbent cost is the major cost driver for solid DAC systems. For example, Bos et al., (2020) reported that sorbent cost represented 73% of the capital expenditure for solid DAC, while Wu et al., (2022) found that sorbent cost was the largest contributor to the capture cost for various solid DAC technologies.

The second largest component of the levelized costs is electricity cost, which represents 21% of the levelized cost. Electricity cost depends on the electricity price and consumption of the DAC process, which are influenced by factors such as sorbent type. Therefore, optimising the energy efficiency of sorbent and utilisation of renewable energy is important for lowering the electricity cost of DAC.

The next component is capital expenditure, which accounts for 9% of the total cost.

The figure also shows that the LCOD and LCOH for this study together are 0.155  $\epsilon$ /kgCO<sub>2</sub>, which is lower than most of the literature values for solid DAC systems. This is because this study assumes that waste heat from industrial sources is used for sorbent regeneration, which eliminates the need for external heat supply. According to IEA, heat accounts for 75% to 80%

of the total energy demand of DAC. Fasihi et al., (2019) performed a techno-economic analysis of DAC considering different scenarios of heat supply. They reported that using waste heat reduced the capture cost from 0.233  $\epsilon$ /kgCO<sub>2</sub> to 0.133  $\epsilon$ /kgCO<sub>2</sub> compared to using low-cost heat. Therefore, using waste heat or performing heat integration is a key factor for achieving a low levelized cost for DAC.

# <span id="page-54-1"></span>3.4. Cost structure of PV-Battery system

PV with battery is a well-known technology and several articles have been found on the cost structure. The major cost driver for PV with battery is the battery costs. In the graph below, the capital expenditure of the PV system is divided into two components: capital expenditure of PV and capital expenditure of battery. The operational expenditure also consists of operational expenditure of PV and operational expenditure of battery. This cost breakdown helps us to show what are the major components involved in the levelized cost of electricity since electricity has been identified as major component for electrolyser.



Figure 9: Levelized cost breakdown OF LCOE

<span id="page-54-0"></span>[Figure](#page-54-0) 9 shows the levelized cost breakdown of electricity (LCOE) for photovoltaic system with battery. The figure indicates that the battery cost is the main component of the LCOE, accounting for 69%. This is followed by the capital expenditure of the photovoltaic system, which represents 31%. Nizami et al., (2022) concluded that methanol production from the PV –battery scenario was higher than that in the PV–grid scenario because of the higher cost of the battery component. [Figure](#page-54-0) 9 also shows that the operational expenditure of the battery and the photovoltaic system are relatively minor contributing to less than 1%. The share of the operational expenditure has been plotted in [Figure 10](#page-55-1) to show which component has the significant share. The figure shows that the battery is till the major component in the operational expenditure of PV system with battery.



Figure 10: Share of operational expenditure of PV system

- <span id="page-55-2"></span><span id="page-55-1"></span>4. Sensitivity analysis
- <span id="page-55-3"></span>4.1. Climate data variation

Relative humidity (RH) is an environmental factor that affects the capture cost of  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$ using solid sorbents. The annual variability of RH in the chosen region is obtained from the NASA data access viewer. The lowest value of RH (10%) is considered as the worst climate case and the highest value of RH (100%) as the best climate case. Table 10 shows the LCOM for the two scenarios under different RH values. [Table 10](#page-55-0) shows the results obtained for the worst and best climatic cases.

<span id="page-55-0"></span>

	<b>RH</b>	<b>LCOM SC1</b>		<b>LCOM SC2</b>	
<b>Base case</b>	70%	$0.63 \text{ E/kg}$	00%	1.25 €/kg	100%
Worse climate case	0%	$0.97 \text{ E/kg}$	$+54%$	$2.13 \text{ E/kg}$	$+70%$
<b>Best climate case</b>	$00\%$	$0.60 \text{ E/kg}$	$-4\%$	.19 €/ $k$ g	$-5%$

Table 10: Sensitivity analysis on Relative Humidity

In the most unfavourable climate, LCOM\_S1 increased by 54% while LCOM\_S2 increased by 70%. This difference is due to the fact that water electrolysis is more sensitive to the cost of  $H_2O$ than  $CO<sub>2</sub>/H<sub>2</sub>O$  co-electrolysis. In the best climatic conditions, there is only a slight decrease compared with the two scenarios. This suggests that the average humidity of 70% in the chosen

region is economically favourable to improving costs. It also suggests that location and climatic conditions can have an impact on the cost structure of e-methanol using solid sorbent direct air capture technology.



The [Figure 11s](#page-56-1)hows the LCOM trend for the two scenarios as a function of relative humidity

Figure 11: LCOM variation with Relative Humidity

### <span id="page-56-2"></span><span id="page-56-1"></span>4.2. Capital expenditure variation for Direct Air Capture

The results of capital expenditure projection for 2050 of direct air capture and the related cost of CO<sup>2</sup> and methanol in [Table 11.](#page-56-0)

<span id="page-56-0"></span>

	LR	b	2020	2030	2040	2050
<b>Production Mtco2</b>	$\overline{\phantom{0}}$			473	4791	15356
Capex $\epsilon$ /tco2	5%	0.23446525	730	222.858509	129.496837	98.54951
LCOD $\epsilon$ /kg	$\overline{\phantom{0}}$	$\overline{\phantom{0}}$	0.08	0.05	0.045	0.043
LCOM_SC1 $\epsilon$ /kg	$\overline{\phantom{0}}$	$\overline{\phantom{0}}$	0.63	0.59	0.58	0.57
<b>LCOM SC2</b> $\epsilon$ /kg	$\overline{\phantom{0}}$		26	1.17	1.15	.14

Table 11: Future cost estimation for direct air capture

With the cost calculated, the sensitivity analysis has now been performed using What if scenario in MS Excel and the results are reported in [Table 11](#page-56-0) and illustrated in [Figure 12.](#page-57-0)



Figure 12: LCOD trend projection with future DAC cost

# <span id="page-57-2"></span><span id="page-57-0"></span>4.3. Capital expenditure variation for SOEC.

SOEC is an emerging technology that has high capital cost and low lifetime compared to other electrolysis technologies. A sensitivity analysis is performed on the SOEC cost to show how it affects the syngas cost and the LCOM. The future cost projections for SOEC capex and stack price from (Salomone et al., 2019) and (Jambur, 2022) respectively is used.



The result of our sensitivity analysis is shown in [Figure 13](#page-57-1) below.

<span id="page-57-1"></span>Figure 13: LCOM trend projection with SOEC capex projection

[Figure 13](#page-57-1) shows the LCOM for scenario 1 under SOEC costs in 2020 and 2050. The results show that with the only SOEC capital cost projection, the levelized cost of methanol has decreased more 16%. This shows the impact of the capital expenditure of SOEC on the overall cost structure. Not only the capital expenditure of SOEC is high, but the stack lifetime is also low compared to PEM and alkaline technology. Future improvement could help improve the stack lifetime and reduce the initial investment of SOEC.

### <span id="page-58-1"></span>4.4. Electricity cost variation

According to Mauler et al., (2021), lithium-ion batteries could reach cost potentials below 90 \$/kWh (78.93€) by 2050 based on a consolidation of 360 data points from 53 studies. Lithiumion battery improvement and future cost estimation has been area of interests of many studies because it is the major cost in PV-battery system. In our study, another estimation will not be done, only the prediction will be taken to analyse the cost of this variable on the final cost of methanol.





<span id="page-58-0"></span>The [Figure 14](#page-58-0) above shows a reduction of more than 33% in the first scenario and 23% in the second scenario for lithium-ion future cost prediction. This is still a bit higher than the current methanol market price of methanol 395  $\epsilon$ /ton provided by Methanex for July to September 2023 (Methanex Corporation, 2023).

<span id="page-59-0"></span>5. Analysis of the value added at each stage of the process.

Each production stage provides advantages and added value to the entire process. Capturing water and carbon dioxide with the solid Direct Air Capture sorbent offers benefits over purchasing raw materials. The captured  $CO<sub>2</sub>$  is carbon negative and can generate carbon credits. Additionally, extracting water averts impacting scarce local water resources. A key economic benefit is selling excess water for agriculture or industry. On-site production of  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$ also avoids transportation costs and emissions associated with procuring these inputs externally. It further stabilizes production expenses by removing market fluctuations in transported fuelbased feedstocks.

The co-electrolysis or electrolysis stage for the production of syngas or hydrogen also offers major economic added value compared with the purchase of these feedstocks. In fact, apart from the carbon footprint associated with transporting these raw materials, it is the oxygen that is produced as a by-product during electrolysis that can be sold to local industries or hospitals.

The production of syngas in scenario 1 also offers the advantage of more efficient use of raw materials and, above all, energy. Given that energy is the main cost driver for production, the final cost of methanol is 50% lower in scenario 1 than in the second scenario. In addition to energy, scenario 1 uses less  $CO<sub>2</sub>$  and  $H<sub>2</sub>O$  than the second scenario. This is normal because the same reactor has an input ratio of 2 if it is fuelled with syngas and an input ratio of 3 if it is fuelled with pure hydrogen mixed with carbon.

<span id="page-59-1"></span>6. Impact of the result on the field of research, society, and economy

For the field of research, the study provides a comprehensive and detailed analysis of the cost structure and value chain of renewable methanol production from direct air capture (DAC) and solid oxide electrolysis cells (SOEC) in an arid region. It shows that using novel co-electrolysis process saves energy and is more economics than PEM methods. The study also identifies the main cost drivers and areas for improvement, such as battery for energy storage, DAC sorbent, and SOEC stack. The study contributes to the existing literature on renewable methanol production and offers insights for future research on sensitive areas to optimize the process and reduce the costs.

For society, the study demonstrates the potential of renewable methanol as a future fuel or feedstock for the chemical industries that can reduce greenhouse gas emissions and mitigate

climate change. The study also shows how renewable methanol production can create carbon credits, water savings, and oxygen surplus that can benefit the local communities and industries in terms of economic and social value. Renewable methanol can also create social benefits, such as job creation, rural development, and public health improvement, by utilising local resources and reducing air pollution.

The study impacts the economy by showing the current economic challenges and opportunities for renewable methanol production using  $CO<sub>2</sub>$  from direct air capture. It reveals that renewable methanol is not yet competitive with conventional methanol or biomass methanol in terms of production cost, but it can be profitable under certain conditions, such as low electricity price, and low capital expenditure for SOEC. The study also suggests that renewable methanol can create economic value by selling excess of  $CO<sub>2</sub>$ , or oxygen to local industries, as well as by receiving carbon credits for capturing and utilizing  $CO<sub>2</sub>$  from air. The study also provides guidance for policy makers and investors to support the development and deployment of renewable methanol technologies and markets.

# Chapter V: Conclusion, Recommendations and Limitation

1. Conclusion

<span id="page-61-1"></span><span id="page-61-0"></span>In conclusion, exploration of the cost structure and value chain of renewable methanol production has shown remarkable future potential for methanol as a future fuel or feedstock for the chemical industries.

The study identified and quantified the different inputs and outputs of each stage of the production chain to answer the first two research questions. The technologies received, as well as their inputs and outputs, allowed a detailed analysis of the cost structure of e-methanol production, providing clear answers to the third research question of our study, namely the identification of cost structure and cost drivers identification.

The detailed analysis of the cost structure in the production chain showed several current economic challenges mainly due to the rather high energy demand from electrolysers and direct water capture technology. The scenario 1 approach with SOEC syngas production is more efficient and consumes not only less energy, but also less water and more  $CO<sub>2</sub>$  than the conventional approach using hydrogen produced by PEM. This results in a difference in the final cost of methanol of almost 50%, i.e. 0.63  $\epsilon$ /kg and 1.26  $\epsilon$ /kg respectively for scenarios 1 and 2.

However, neither scenario is competitive with the current market price of methanol or the cost of producing methanol from biomass. The cost drivers identified are sorbent costs for DAC and capital costs for DAC. Sorbent alone represents almost  $63\%$  of the levelized cost of  $CO<sub>2</sub>$  and water. The second important point is the capital cost of the SOEC and the cost of replacing the stack. Sensitivity analysis has shown a reduction of 17% in the cost of syngas and 16 % of the final methanol cost with the future projection of the SOEC capital cost. The final and most important cost driver is electricity, which is what makes syngas,  $H_2$ ,  $CO_2$  and  $H_2O$  feedstocks so expensive. The cost of electricity is driven by the cost of the battery with a share of 69%. These points, namely battery, DAC sorbent and its absorption capacity, SOEC and its stack lifetime, represent areas for improvement in future research to make renewable methanol more economical and competitive.

A study of the value added at each stage of production shows that the  $CO<sub>2</sub>$  produced on site presents a carbon credit opportunity. Also, the water needs are covered directly by the DAC which gives a negative water footprint for this production method. In the first scenario, excess water can be sold or donated to a neighbouring community. In the second scenario, the excess

CO<sup>2</sup> can be sold to local industries to offset the total cost of methanol production. The electrolysis stage in both scenarios produces oxygen which can be sold to local hospitals or industries to also amortise the cost structure of producing the final product positively.

2. Recommendations

<span id="page-62-0"></span>To reduce costs and improve the feasibility of renewable methanol production via power-tomethanol, the following recommendations are made:

- To increase cost-effectiveness and efficiency, research and development should focus on optimising direct air-capture sorbent materials and SOEC stack.
- Working with battery experts to develop more cost-effective high-capacity storage options would lower process electricity costs.
- Carbon pricing and renewable energy credits, for example, can assist in bridging economic disparities during initial deployment and technology scale-up.
- Fostering collaboration between academic, industrial and government partners through joint research initiatives that can holistically optimise the production process.
- Conducting comprehensive life cycle and environmental impact assessments would quantify benefits and could motivate further support through improved incentives.
- Investing in pilot and demonstration scale production facilities can help drive down costs through learning-by-doing and economies of scale. The knowledge gained can inform further scale-up.
- Consumer demand and uptake could be boosted by public awareness campaigns emphasising the environmental benefits of renewable methanol over its fossil fuel-based counterparts.
- Exploring business models like methanol-as-a-service, which separate operating costs and investment costs, could reduce risk for investors and enable adoption by smaller operators.

# 3. Limitation of the study

<span id="page-63-0"></span>This study has some limitations that should be acknowledged and addressed in future research. These limitations are:

- Data availability: Primary data on the technologies were not available to design the plant used in this study. Instead, secondary data from the literature, which may have different assumptions and uncertainties have been used.
- Maturity level of SOEC: SOEC is a technology that is still at the lab scale, with many uncertainties on its performance and cost. Future cost projections used is taken from the literature, which may not reflect the actual cost reduction and learning rate of SOEC.
- Time limitation for the research: this study is conducted within a limited time frame, which restricted the scope and depth of our analysis. A comprehensive sensitivity analysis could not perform on all the parameters and scenarios considered in this study.
- Scope of the study: Only the production stage of e-methanol using solid sorbent DAC and PV system has been the interest of this paper. Other stages of the methanol value chain, such as transportation, storage, distribution, and end-use are not considered. These stages may have different economic impacts on the cost structure that should be considered in a full life cycle assessment.

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