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Carbon capture and storage through molten carbonate fuel cells systems:

feasibility study and optimization through simulation and experimental work

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CARBON CAPTURE AND STORAGE THROUGH MOLTEN CARBONATE FUEL
CELLS SYSTEMS:

FEASIBILITY STUDY AND OPTIMIZATION THROUGH SIMULATION AND
EXPERIMENTAL WORK

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Abstract

This thesis investigates Molten Carbonate Fuel Cells (MCFCs) as a dual-purpose technology uniquely capable of simultaneously generating electricity and capturing carbon dioxide (CO₂). This intrinsic feature makes MCFCs a highly promising solution for carbon mitigation.

The research focuses particularly on their potential application within the maritime sector and aligns with the increasing global drive toward decarbonisation, supported by new regulatory frameworks such as the International Maritime Organization (IMO) directives, the European Union Emissions Trading System (EU ETS), and FuelEU Maritime, which are setting ambitious CO₂ reduction targets and imposing carbon costs.

The work has been developed along two complementary research paths: an experimental investigation and a system-level analysis.

From the experimental perspective, the study focused on the development and characterization of key MCFC components, with particular attention to identifying manufacturing routes suitable for future industrial scale-up. In particular, the matrix, that is a crucial element that separates the electrodes and hosts the electrolyte, enabling ion transport, was optimized to achieve competitive performance using environmentally compatible materials and an innovative formulation was designed and produced.

All fabrication and testing activities were carried out within the Caplab laboratory, a joint research facility between the University of Genoa and the company Ecospray Technologies, and further performance assessments were conducted at the Royal Institute of Technology (KTH) in Stockholm during an international research period. The performed tests achieved power densities higher than values typically reported in the literature, thereby confirming the effectiveness of the developed materials and fabrication procedures.

From the system-level standpoint, a simulation-based study was performed to explore the integration of MCFC technology within Onboard Carbon Capture and Storage (OCCS) systems. Starting from literature-based layouts, several improvements and process optimizations were introduced, including gas recirculation strategies. A comparative analysis based on key performance indicators (such as electrical efficiency, fuel demand, system complexity, and spatial requirements) highlighted the strengths and trade-offs of different configurations, considering different net CO₂ capture rates.

Finally, the applicability of MCFC-based systems was evaluated for carbon-intensive industrial sectors, such as steel production, to assess their performance when treating carbon-rich off-gases under oxygen-deficient conditions.

Overall, this thesis demonstrates the potential of MCFC technology as a promising solution for carbon capture and energy conversion, combining experimental advances in sustainable materials with system-level insights that pave the way for future large-scale applications.

Acronym	Definition
CCS	Carbon Capture and Storage
OCCS	On-Board Carbon Capture and Storage
SMR	Steam Methane Reforming
DBP	Dibutyl Phthalate (plasticizer)
DMR	Dry Methane Reforming
eSMR	Electrically Heated Steam Methane Reformer
EU ETS	European Union Emissions Trading System
FuelEU Maritime	EU regulation setting greenhouse-gas intensity limits for maritime fuels
GC/IR	Gas Chromatography / Infrared Spectroscopy
HFO	Heavy Fuel Oil
IMO	International Maritime Organization
LNG	Liquefied Natural Gas
MCFC	Molten Carbonate Fuel Cell
SEM	Scanning Electron Microscopy
PLC	Programmable logic controller

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1 Introduction

Maritime transport is a critical component of the global economy, responsible for the movement of approximately 90% of international trade by volume [1]. It is of the utmost importance for growth, as it enables large-scale goods trade across the globe. However, the environmental impact this market has must not be understated. The sector accounts for approximately 3% of global Greenhouse Gas (GHG) emissions [2].

Therefore, actions must be taken to counteract this, as both social and economic pressure are increasing on actors inside the market. With international accords like the Paris Agreement [3] setting the stage for a global push towards decarbonisation of all sectors, the maritime sector is now also starting to introduce its regulations through the International Maritime Organization (IMO) rulings, that require a significant reduction of vessel emissions and the introduction of the shipping sector into the Emissions Trading System (ETS) [4], [5]. These new regulations are in strong contrast with the past of the shipping sector, as it has previously been exempted for the most part from the international push towards decarbonisation. This means that the main market players are now searching for new solutions for this issue and are incentivised to do so, contrary to how it was in the past.

1.1 Impact of carbon emissions on the environment

Whilst it is generally recognised that the maritime sector has the lowest ton-per-kilometre carbon emissions amongst the most common transportation means [6], it is also true that through the volume of sea trade, the emissions sum up to significant numbers. As mentioned before, the sector is responsible for 3% of the global GHG emissions and is projected to increase further in the coming years [7], and it accounted for 1.056 million tons of CO₂ in 2018.

The cause for these strong emissions can be found in the fuel used on board of vessel, being primarily Heavy Fuel Oil (HFO) [8]. This HFO is a heavy fraction obtained during the refinement of crude oil; it therefore contains fractions of various pollutants. The combustion of HFO produces various dangerous substances apart from CO₂. Nitrogen oxides (NO_x), sulfur oxides (SO_x), methane (CH₄), particulate matter (PM), and black carbon, all of which have negative effects on health, environment, and air quality, particularly in port cities. It is estimated that between 60.000 to 100.000 deaths yearly in port and coastal regions are caused by the effects of these gases on the human body [9]. They can cause the onset of respiratory and cardiovascular conditions. With the sector projected to grow, the number of people affected is also set to increase [9]. Beyond the localised effect of these pollutants, they also contribute to the overall global warming. CO₂ is a well-known contributor to global warming because of its long term accumulation potential inside the atmosphere [10], while others, like carbon black, can have more niche effects, as they increase the melting speed of the polar regions by depositing on the ice and thus reducing the reflectivity of the ice itself, causing it to heat faster and disrupting the climate [11].

Looking back at the sector specific risks, the CO₂ emissions in the maritime sector are also a driver towards the acidification of the sea. The CO₂ can dissolve in the water and form carbonic acid (H₂CO₃), which affects the pH of the sea water, and therefore can also have an impact on the maritime environment [12]. It is evident that an effort towards the reduction of emissions in the maritime sector is of primary importance and can also be a chance to stride towards new technologies which might also improve the overall efficiency of the shipping sector.

1.2 Legislations

After recognising the urgent need to cut carbon emissions, new legislations are being introduced to encourage the sector to step up its decarbonisation efforts. Since this is a global challenge, regulations are also being developed at the international level. For instance, while the EU and the US have adopted different approaches, both are working toward similar climate goals.

1.2.1 International Maritime Organisation (IMO)

The IMO is a specialized agency of the United Nations responsible for regulations in the shipping sector, and it has long played a central role in addressing maritime safety and emission reduction. It is the globally recognized main regulating body in the field, and it is therefore responsible for shaping the direction the shipping sector is heading in through its legislations. The main regulations that have tackled the emission issue in the past are listed in chronological order in the following section.

The IMO's first significant step toward environmental protection came in the form of the International Convention for the Prevention of Pollution from Ships (MARPOL), adopted in 1973 and modified by the MARPOL 1978 Protocol. Annex VI of this convention, introduced in 1997 and enforced starting in 2005, specifically targets air pollution from ships, setting limits on NO_x and SO_x emissions and introducing global caps on sulphur content inside fuels [13]. In 2011, the IMO introduced the Energy Efficiency Design Index (EEDI) [14], the first legally binding climate change measure mandating improved efficiency in newly built vessels. This was complemented by the Ship Energy Efficiency Management Plan (SEEMP) [15], which requires all ships to implement onboard management plans to monitor and improve energy efficiency. These were of primary importance to allow the subsequent introduction of more stringent regulations, as it started giving overview on what is happening inside the vessel environment. The most significant development came in 2018, when the IMO adopted its Initial GHG Strategy. This landmark agreement set a goal to reduce total annual GHG emissions from international shipping by at least 50% by 2050 compared to 2008 levels, while aiming to phase them out entirely within this century. Importantly, the strategy calls for the development and implementation of a revised strategy by 2023, incorporating more ambitious intermediate targets [4]. In 2023, the IMO reinforced its commitment by adopting measures to activate the Carbon Intensity Indicator (CII) and updated requirements for SEEMP. These measures rank ships based on their carbon intensity, assigning grades from A to E. Ships receiving a D or E grade for three consecutive years must implement corrective actions or they receive compliance penalties [16]. Whilst many regulations were introduced, IMO faced significant backlash throughout the years because these regulations were often seen as inadequate to counteract the issue

and had significant loopholes and regulatory voids that allowed the shipping sector to be mostly untouched by significant changes [17].

1.2.2 IMO Net-Zero Framework (2025)

IMO introduced this new regulation in 2025, marking the beginning of a new regulatory period, that sets a clear target and clear incentive towards decarbonising the maritime sector. The base of the framework is the introduction of a global carbon pricing mechanism. From 2027 onward, ships emitting CO₂ above a defined baseline will be subject to a carbon penalty of USD 100 per metric tonne of CO₂. This unified cost allows other alternative technologies to have a benchmark that they need to strive for to be competitive in the field. In parallel, the IMO has adopted emission intensity standards targeting marine fuels. These standards mirror similar mechanisms in aviation and road transport, establishing maximum carbon intensity values for marine energy sources. The built in steps that make the regulations more stringent over time have the aim to force a transition towards greener fuels or the electrification of the vessels. The framework also introduces a mandatory GHG reporting and verification protocol. Building on the Data Collection System (DCS) for fuel oil consumption, ships must now report GHG emissions verified by a third-party. Compliance is enforced through audits and port control inspections, with non-compliant vessels subject to fines, restrictions, or detentions. A key aspect of the Net-Zero Framework is that it applies not only to vessels, but also to the wider port infrastructure, which needs to be able to sustain the drive towards decarbonisation. This is achieved through guidelines that define the technical and operational requirements ports must meet, such as the capability to store and handle alternative fuels, provide shore-side electricity, and manage products generated by onboard carbon capture systems. Overall, the framework provides a clear regulatory signal to the sector by embedding science-based criteria, thereby reducing ambiguity and limiting discretionary interpretation. The success of these rulings will be determined based on how the international political landscape will decide to implement them into their own local national laws, but they signal a step in the right direction [18].

1.2.3 European Union's Emissions Trading System (EU ETS)

The European Union (EU) has always led the push towards decarbonisation, with regulations and innovations. In 2005, the EU ETS system was introduced, initially to counteract the emissions of power plants and industrial facilities. This system assigns, similarly, to what was previously discussed for the Net-Zero Framework, an economic value to emissions, giving an incentive to the reduction of CO₂ emissions. In 2024, this system was expanded to the maritime sector, marking the first financial incentive in this market towards decarbonisation. In the maritime application, vessels above 5,000 gross tonnage conducting voyages within the EU, as well as between EU ports and external ports, are required to purchase and surrender allowances equivalent to their verified emissions. The implementation follows a phased approach: 40% of emissions are covered by 2025, rising to 70% by 2026, and reaching full 100% coverage by 2027. This step-based introduction is aimed at allowing the targeted vessels to adapt to the new regulations. The ETS operates under a “cap and trade” principle: the total number of emission allowances is capped and reduced annually, driving the prices of the

allowances up. Companies that reduce emissions can sell excess allowances, while those that exceed their caps must purchase more. This market-driven system creates a financial cost for pollution, encouraging innovation and operational efficiency. For shipping companies, this means investments in cleaner engines, energy-saving technologies, and low-carbon fuels become more economically attractive as time goes on, and can, if done correctly, bring even a net profit throughout the transition.

Administrative responsibility for compliance lies with the shipping companies, which must monitor and report emissions under the Monitoring, Reporting and Verification (MRV) regulation. The European Maritime Safety Agency (EMSA) plays a key role in overseeing the system and ensuring data integrity. Penalties for non-compliance include fines, exclusion from EU ports, and restrictions on operational licenses [19], [20].

1.2.4 FuelEU Maritime Regulation

In alignment with the European Union's broader climate ambitions, the FuelEU Maritime Regulation serves as a key policy mechanism parallel to the extension of the EU ETS to the maritime sector. Adopted in 2023 and entering into force in January 2025, the regulation imposes limits on the GHG intensity of the fuel used onboard vessels, pushing the industry toward a gradual and sustained adoption of low-carbon content and renewable fuels [21]. The regulation is applicable to ships above 5,000 gross tonnages reaching EU ports, independently of the flag they travel under. It mandates a gradual reduction in the GHG intensity of the fuels used onboard, starting with a 2% cut in 2025 relative to a 2020 baseline and increasing progressively to 80% by 2050 [22]. This allows for a gradual but decisive movement towards the carbon neutrality on a long-term basis. What makes EU Fuel special is its flexibility towards carbon neutral fuels, as rather than prescribing specific energy types, the regulation allows shipowners to choose from a range of compliant fuels, including advanced biofuels, e-methanol, green ammonia, hydrogen, and renewable LNG. This flexibility supports technological innovation and enables operators to select options best suited to their routes, cargo types, and vessel configuration. The European Union requires every vessel to undergo a yearly review by an independent third party. Vessels that don't comply incur into possible financial punishment. Another notable provision is the *pooling mechanism*, which enables ships under the same operator or within a fleet to aggregate and average their GHG-intensity performance. This approach incentivizes early investment in zero-emission or near-zero-emission vessels while offering compliance flexibility to operators managing heterogeneous fleets, thereby lowering exposure to non-compliance and penalty risk. From an economic perspective, the regulation is expected to reshape fuel supply chains and influence ship and propulsion system design. Although the transition may raise operating costs in the short term, it simultaneously creates market opportunities in renewable and low-carbon fuel production, bunkering logistics, and retrofit activities across shipyards and the wider maritime value chain. Ultimately, if implemented coherently, the combined effect of the EU ETS and FuelEU Maritime can strengthen decarbonization incentives and accelerate progress toward the EU's long-term zero-emission objectives.

1.3 Solutions to be regulation compliant

From the discussion had in the previous section, the need to reduce emissions is evident, both from an environmental and economic perspective. It is now of interest to analyse what options are available and discuss the possible technologies that actors in the sector can take. The last solution, being Carbon Capture and Storage (CCS), will be discussed in a separate chapter, given its central role inside the present work.

1.3.1 Alternative Fuels

HFO is, as of now, still the most used fuel in maritime faring, with the issues connected with it [23]. The first step towards a decarbonisation process is cutting down on these carbon-intensive fuels and approaching alternatives. Amongst these, some of the most promising are discussed in the following section:

- **Liquefied Natural Gas (LNG):** LNG is often seen as a transition fuel. This is because it is still carbon-based, but it cuts down on most of the other pollutants that are present in HFO, like NO_x , SO_x and particulate matter. What makes LNG great is its high power density of 55 MJ/kg compared to HFO, which is around 41 MJ/kg [24], [25]. Furthermore the carbon content, expressed as carbon factor ($\text{tCO}_2/\text{tFuel}$) is lower compared to HFO, as it reaches 2.75 compared to HFO 3.114 [26].
- **Green ammonia (NH_3):** Green ammonia is produced using renewable sources of hydrogen and nitrogen and is of interest as its combustion does not release carbon. Although it has a lower energy density compared to its fossil counterparts (18.56 MJ/kg) it is often considered as it has a higher volumetric density than hydrogen, which it can carry [27]. Despite significant challenges associated with toxicity, corrosivity, and stringent storage and handling requirements, green ammonia remains a promising option for large-scale hydrogen transport and as a candidate fuel for low-carbon maritime applications [28].
- **Hydrogen (H_2):** Hydrogen is attracting substantial interest across multiple industrial sectors, including maritime transport. Green hydrogen is regarded as a highly promising zero-emission energy carrier, as its use produces no direct CO_2 emissions. However, its deployment is constrained primarily by its very low volumetric energy density, which imposes significant space penalties onboard, and by the stringent storage requirements, most notably cryogenic containment for liquid hydrogen to achieve practicable energy densities (temperatures around 20 – 110 K and pressures that range from 0.2 – 80 mPa [29]) and safety-related issues, as it can form explosive mixtures in air.
- **Methanol (CH_3OH):** Methanol (and its bio counterpart) is very interesting because of the ease of handling, when compared to ammonia, hydrogen, or even LNG. It can be produced renewably through biomass gasification or even through captured CO_2 [30]. Yet, the combustion is still forming CO_2 , and its application can therefore still only be considered as a transition fuel. It is also often considered thanks to its very low carbon factor of 1.375 compared to HFO (3.114) [31].

There is not a universal optimal solution, but every case requires further investigations to find the best option. Furthermore, the option of utilising dual fuel engines is also of market interest as it gives the possibility to go through a softer transition period and more efficient combustion [32], [33], [34].

1.3.2 Design optimisation

The vessel design itself can majorly contribute to reducing the amount of fuel required, and this, in turn, reduces the emissions. Amongst the possible optimisations, the following are the most promising:

- Hull optimisation: This involves streamlining the design of the hull and applying different kinds of lubrication systems, all aimed at reducing the hydrodynamic drag of the vessel in the water and therefore reducing the power requirement for movement [35].
- Propulsion improvement: The introduction of design optimization of propellers and shaft generation to allow for energy recovery all improve the overall vessel efficiency [36], [37].
- Wind-Assisted Propulsion: While less widespread, modern sail and rotor systems can harness wind energy, and, if optimised and integrated with the engine, it is possible to reduce engine loads [38], [39].
- Waste Heat Recovery: The engines have a lot of waste heat that is available towards the vessel environment, and recovering this heat allows for cogeneration of steam, or in some cases even hydrogen [40].

1.3.3 Digitally aided optimisation

Through the employment of advanced software and the introduction of artificial intelligence, different optimisation routes have been opened that were previously undiscovered, amongst these, the most promising are:

- Voyage Optimisation: Through the analysis of weather patterns, currents, and cargo, it is possible to determine the most fuel-efficient routes [41].
- Fleet Management: As discussed before, vessel performance can be expanded towards a more globalised vision of the whole fleet, at least in terms of legislation. The ability to monitor all vessels inside a fleet in real time allows for finding bottlenecks and optimizing each vessel accordingly [42].
- Predictive Maintenance: With advanced sensors and machine learning capabilities, it is possible to anticipate the degradation and failure of vessel equipment. By doing this, it is possible to operate at peak efficiency for longer times, reducing consumption caused by degradation [43].

1.4 Aims and objectives

The aim of this PhD thesis is to evaluate Molten Carbonate Fuel Cells (MCFCs) as a dual-function technology enabling simultaneous electricity generation and CO₂ capture, with a primary focus on OCCS in the maritime sector, done through a coupled experimental and system-level simulation approach.

To reach this aim the following objectives have been set:

1. Develop and optimise MCFC components for carbon capture-oriented operation, with particular focus on the MCFC matrix, and study fabrication routes compatible with future industrial scale-up and environmentally compatible material choices.
2. Establish a reproducible fabrication and characterisation workflow for the produced components, linking the microstructure to functional requirements such as electrolyte retention, ionic transport and mechanical integrity, through extensive comparison with literature. Porosity and pore size have been determined to be of primary importance with target values of around 50 - 70% and $< 1 \mu\text{m}$ respectively for the matrix, 55% and $3 - 6 \mu\text{m}$ respectively for the anodes and 60- 65% and $6 - 12 \mu\text{m}$ respectively for the cathode.
3. Experimental validation of electrochemical performance benchmarking the developed components against literature targets and confirming repeatability through testing in an external setup. The targets that have been set are a power density of 120 mW/cm^2 and an OCV of 1.23 V.
4. Adapt an existing MCFC model to a new process-simulation environment (DWSIM), ensuring consistency of the electrochemical logic and enabling full system mass and energy balances for OCCS integration studies.
5. Design and optimise MCFC-based OCCS system configurations for ships, starting from literature layouts and introducing process modifications to improve net CO₂ capture performance and reaching targets compatible with the legislative underlying framework.
6. Compare alternative configurations through quantitative Key Performance Indicators (KPI), including net CO₂ capture rate (20–80% target range where achievable), specific fuel consumption (kgLNG per tCO₂ captured) energy and fuel efficiency, and indicators of shipboard feasibility such as system complexity (units and recycles) and footprint.
7. Assess transferability to industrial carbon-rich off-gas applications, applying the same modelling framework to a real case study to discuss opportunities and limitations beyond the maritime context.

2 Introduction to CCS technologies

With the increasingly stringent regulations mentioned in the previous chapter, Carbon Capture and Storage (CCS) is increasingly recognized as a critical mitigation strategy. Although CCS technologies differ widely in design and application, they share a common goal: capturing and securely storing CO₂ emissions. This technological diversity reflects the varying nature of emission sources. For example, the composition and flow of emissions from industrial smokestacks differ considerably from those produced by internal combustion engines, requiring customized capture approaches.

This work focuses specifically on a subset of CCS, Onboard CCS (OCCS), which presents unique challenges compared to land-based systems. While the emphasis will be on post-combustion capture methods, it is worth noting that CO₂ can also be captured through pre-combustion techniques, depending on the system configuration and fuel type.

2.1 OCCS technologies

Exhaust gases from the engines of vessels are quite diverse, depending on the carbon intensity of the used fuel, yet, it can be said that the tenor of CO₂ inside the gases in terms of overall volume, is lower than industrial off gases. In the case of the vessel exhaust a reasonable value is around 5% vol as the combustion is less pushed [44], whilst other industries using blast furnaces and cement kilns can reach up to 40% vol [45]. This means that the technology needs to be able to work at low percentages of CO₂. The main once will be explained in the following paragraphs and the results compiled in Table 2-1.

2.1.1 Adsorption

Adsorption-based CCS uses solid sorbents, amongst which are zeolites, activated carbons, or metal-organic frameworks (MOFs), to bind CO₂ from flue gas via physisorption or chemisorption selectively. The process typically operates cyclically using Temperature Swing Adsorption (TSA), Pressure Swing Adsorption (PSA), or Vacuum Swing Adsorption (VSA) to regenerate the sorbent [46]. Capture efficiencies vary depending on operating conditions and sorbent properties, but generally fall within the 50–85% range [47]. In shipboard applications, adsorption is promising due to its potentially lower thermal energy requirements (relative to chemical absorption) and modularity. However, adsorption systems are challenged by limited CO₂ capacity, sensitivity to moisture, and sorbent degradation over time [48]. The operative cost estimate for this technology is around 175 - 250\$/t_{CO2Captured}[49], [50].

2.1.2 Membrane separation

Membrane-based CCS offers a compact and modular alternative for post-combustion applications. These systems operate via selective gas permeation through polymeric or inorganic membranes, with separation driven by partial pressure differences. CO₂ capture efficiencies for membrane systems reach up to 90%, depending on membrane material, stage configuration, and flue gas composition [51]. In ship-based applications, membranes are particularly attractive due to their relatively low footprint and mechanical

simplicity. However, the separation of CO₂ from dilute flue gas, as is the case on-board, requires either multi-stage setups or vacuum and purge operations, which increase the energy penalty and auxiliary power demand. Costs vary widely but are estimated at around \$310–350 /t_{CO₂Captured}, depending on membrane performance and system integration [52], [53].

2.1.3 Cryogenic Separation

This technology capitalizes on the fact that CO₂ liquefies at higher temperatures than other flue gas components. This method involves cooling the gas stream to temperatures below -78.5°C , allowing CO₂ to condense or de sublimate for subsequent collection. The process can achieve high CO₂ purities (often >99%) and capture efficiencies over 90%, but it is extremely energy-intensive, particularly when treating low-pressure and low-concentration CO₂ flue gas [52], given the huge volumes of residual components present in the gas mixture. While theoretically viable, the cost for the cooling of high volumes of flue gases, connected with the necessity for strong insulation, makes the on-board application challenging. The cost of capture with this technology on the other hand is around 55 - 130\$/t_{CO₂Captured} [54].

2.1.4 Chemical absorption

Chemical absorption remains the most established and commercially ready post-combustion CO₂ capture technique [55]. Solvents such as Mono Ethanol Amine (MEA), piperazine, and Methyl Di Ethanol Amine (MDEA) are employed to react chemically with CO₂ in the absorber, with the solvent then regenerated in a reboiler. Capture efficiencies typically reach 85–90%, with MEA requiring reboiler duties of 3.5–4.5 MJ/kg CO₂ [56]. While effective, MEA is energy-intensive and degrades over time, creating operational and environmental concerns. In maritime settings, MEA-based systems increase fuel use by 6–12% due to additional heat demand, and total capture costs are estimated between €130–290 per ton CO₂, depending on integration and fuel type [57], [58], [59].

2.1.5 MCFC

MCFCs offer a promising alternative for OCCS by combining capture with power generation. Operating at high temperatures ($\sim 650^{\circ}\text{C}$), MCFCs use a molten carbonate electrolyte to facilitate electrochemical reactions that both generate electricity and capture CO₂ from exhaust gases. MCFC systems can achieve capture efficiencies of up to 90% [60], reducing emissions while offsetting the energy penalty typical of post-combustion technologies. FuelCell Energy reports capture costs as low as \$33.63 per ton CO₂, significantly below those of amine-based systems [61]. While initial capital costs are high due to system complexity and material requirements, the ability to co-produce power and comply with emission regulations supports long-term economic viability.

Table 2-1 Reassessing table of possible post combustion CCS technologies, that can be applied or found on board. The TRL reference both on board and on land applications [62], [63], [64]. Values depend strongly on CO₂ concentration, scale, and system boundaries. *Since no cost-data are currently available for MCFC-based CO₂ capture in onboard applications, the value reported in this work is taken from the corresponding onshore literature and should be regarded as indicative only.

Technology	Cost per Ton CO ₂ avoided (CAPEX + OPEX)	CO ₂ Capture Rate (%)	Advantages	Disadvantages	TRL
MCFC	\$33-91/ton (€30-85 approx.) *	Up to 90%	- Generates power while capturing CO₂ - High integration potential - Compatible with multiple fuels (e.g., LNG, H₂)	- High capital cost - Complex system integration - Durability and maintenance concerns	6
Adsorption	\$175-250/ton	50-85%	- Low thermal energy demand - Modular and compact design	- Sensitive to moisture - Sorbent degradation over cycles - Lower throughput	9
Absorption (MEA-based)	\$130-290/ton	70-90%	- Technologically mature - Widely tested and available - High efficiency	- High energy use for solvent regeneration - Solvent degradation and corrosion issues	7 - 9
Cryogenic Separation	\$ 55-130/ton	Up to 95%	- Produces high purity CO₂ (>99%) - No chemical solvents required	- High electricity demand - large footprint - Inefficient for dilute CO₂	3 - 7
Membrane Separation	\$310-350/ton	60-90%	- Lightweight and modular - No chemicals involved - Easy scalability	- Requires multiple stages - Sensitive to fouling - Efficiency drops with low CO₂ concentration	5 - 7

2.2 Storage and utilisation

Following OCC, several storage and utilization pathways for CO₂ have been proposed to accommodate the operational and spatial constraints of maritime applications. The most established method is liquefied CO₂ storage, where the captured gas is compressed and cooled to approximately 15 – 25 bars, reducing its volume by more than 500 times and enabling compact storage in cryogenic tanks [65]. However, the process is energy-intensive, and the high-pressure, low-temperature conditions require stringent safety measures [66]. An alternative is dense-phase storage, which involves storing CO₂ in a supercritical or dense liquid state within LNG tanks. While this approach lowers energy demand by about 7% compared to full liquefaction and can exploit existing infrastructure, its volumetric capacity is often insufficient for the total CO₂ captured over long voyages [67].

A different approach involves chemical conversion of CO₂, particularly via reaction with calcium hydroxide to form stable calcium carbonate (limestone). This method eliminates the need for gaseous storage and allows for either onboard containment or safe discharge into the marine environment, subject to regulatory compliance. It also presents potential for valorisation, as limestone is a commercially valuable byproduct. However, the process requires substantial quantities of reactive material (approximately 3.19 kg of Ca(OH)₂ per kg of CO₂) and involves additional emissions if the precursor material is not sustainable [68].

Lastly, onboard utilization options such as employing CO₂ as a fire suppressant in engine rooms are being studied as a possible way of carbon capture and utilisation. Although promising, such uses are currently limited in scope and technology readiness, and its future evolution remains to be seen [69].

3 Introduction to MCFC

Among the various technologies within the broader field of CCS, this thesis focuses primarily on MCFCs. MCFCs present a particularly compelling option because they address one of the major drawbacks of conventional CCS systems: high energy demand. Unlike traditional methods that require significant external energy input, MCFC-based systems can generate their own energy through the electrochemical reactions occurring within the fuel cell. This dual functionality, simultaneous CO₂ capture and power generation, makes MCFCs a promising solution for more efficient and self-sustaining carbon capture.

3.1 MCFC

Molten Carbonate Fuel Cells are classified as high-temperature fuel cells, operating at an average temperature of around 650°C and at low pressure, around atmospheric. What sets them apart from other types of fuel cells is their three-phase boundary layer operating principle. At this elevated temperature, the electrolyte, a molten carbonate salt, exists in a liquid phase, enabling ion transport within the cell. To contain the liquid electrolyte and maintain separation between the anode and cathode compartments, a porous ceramic matrix is used. This solid-state component provides structural support while allowing ionic conductivity. The electrodes themselves are nickel-based, acting as catalysts for the electrochemical reactions, while the actual reactants are gaseous. On the cathode side, oxidant gases introduced. On the anode side, a fuel is supplied, usually a hydrogen-rich gas stream. Importantly, this stream can also contain carbon monoxide (CO), which is internally converted to hydrogen via the Water-Gas-Shift (WGS) reaction within the fuel cell, further enhancing fuel utilization and CO₂ capture efficiency [70].

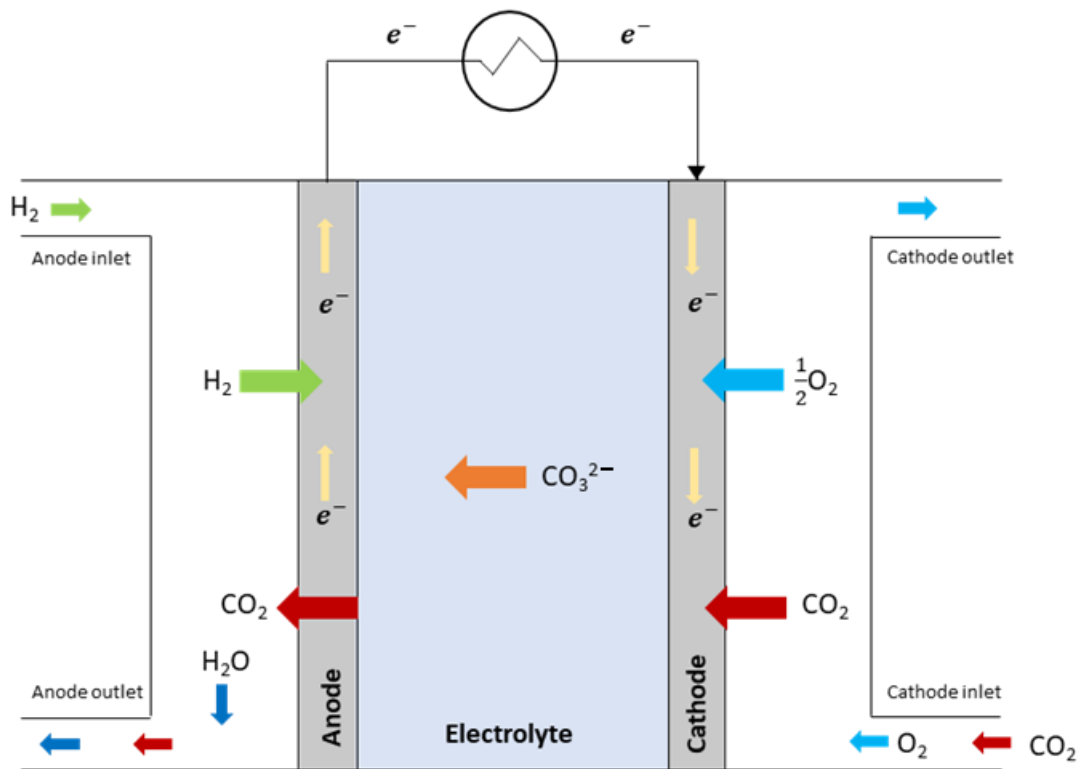


Figure 3-1 Working principle of the molten carbonate fuel cell (MCFC)

The chemical reactions that take place during the process described in Figure 3-1 inside the cell are as follows:

Cathode:	$0,5 O_2 + CO_2 + 2e^- \rightarrow CO_3^{2-}$	<i>Half-cell reaction 1</i>
Anode:	$H_2 + CO_3^{2-} \rightarrow H_2O + CO_2 + 2e^-$	<i>Half-cell reaction 2</i>
Complete reaction:	$H_2 + 0,5 O_2 + CO_{2\ cat} \rightarrow H_2O + CO_{2\ an}$	<i>Complete reaction 3</i>

CO₂ is effectively separated from the air stream as it migrates from the cathode to the anode side of the cell. As a result, the anode exhaust primarily consists of unreacted hydrogen, steam, and concentrated CO₂. This composition enables a simplified separation process: first, a condensation unit can be used to remove water, followed by a cryogenic unit to liquefy CO₂ more efficiently, given the reduced volumes compared to direct exhaust gas liquefaction. Unlike untreated exhaust, which still contains large amounts of nitrogen and oxygen, the MCFC anode stream is already enriched in CO₂. This not only simplifies the liquefaction process but also lowers the overall energy demand, which can be partially offset by the electricity generated by the fuel cell itself.

The cell as described before, has different important components, that have all been studied in this thesis. To be able to better compare the results that have been obtained a literature review for the state of art of each component has been made.

3.2 Matrix

The matrix in an MCFC serves to retain the molten carbonate electrolyte while providing gas separation between the anode and cathode compartments. It must exhibit chemical stability, thermal compatibility, and mechanical strength under operational conditions (~650°C).

The most commonly used matrix material is γ -lithium aluminate (γ -LiAlO₂), favoured for its chemical inertness, high melting point, and compatibility with the molten carbonate mixtures (typically 38/62% Li₂CO₃/K₂CO₃ or 52/48% Li₂CO₃/Na₂CO₃) [71].

3.2.1 Physical characteristics

Different physical properties must be considered to allow for an optimal matrix performance to be reached, mainly porosity, pore size and surface area. These three are responsible for the capacity of the cell to be able to efficiently allow for the passage of ions while providing a good separation of the gas compartments. To do that, literature suggests:

- Porosity: The porosity is usually kept in a range between 30 – 70%. This value is a compromise that allows the matrix to provide sufficient gas separation between the anode and the cathode, while still having enough empty space that can be filled with the electrolyte [72], [73].
- Pore size: The optimal pore size is below 1 micron, this value allows to obtain a strong capillarity effect while not compromising the separation between anodic and cathodic compartment [74].
- Surface area: The surface area is important to allow the formation of a good triple-boundary-layer and is often evaluated at around 10 m²/g. It is possible to find even higher values around 12 m²/g for high performance matrixes although this might cause a reduction in overall lifetime [71].

3.2.2 Fabrication

The fabrication of the matrix itself is subject to extensive investigation, as it plays a critical role in the performance of molten carbonate fuel cells. The process, shown schematically in Figure 3-2, typically involves multiple stages of ball milling, followed by a tape casting step to achieve the desired structural and functional properties. During ball milling, the constituent components, commonly including ceramic powders, plasticizers, binders, solvents and various additives, are thoroughly mixed. These additives are selected to enable precise control over key parameters such as pore size distribution, particle dispersion, and mechanical integrity of the final matrix. The main recipes found in literature can be found in Table 3-1.

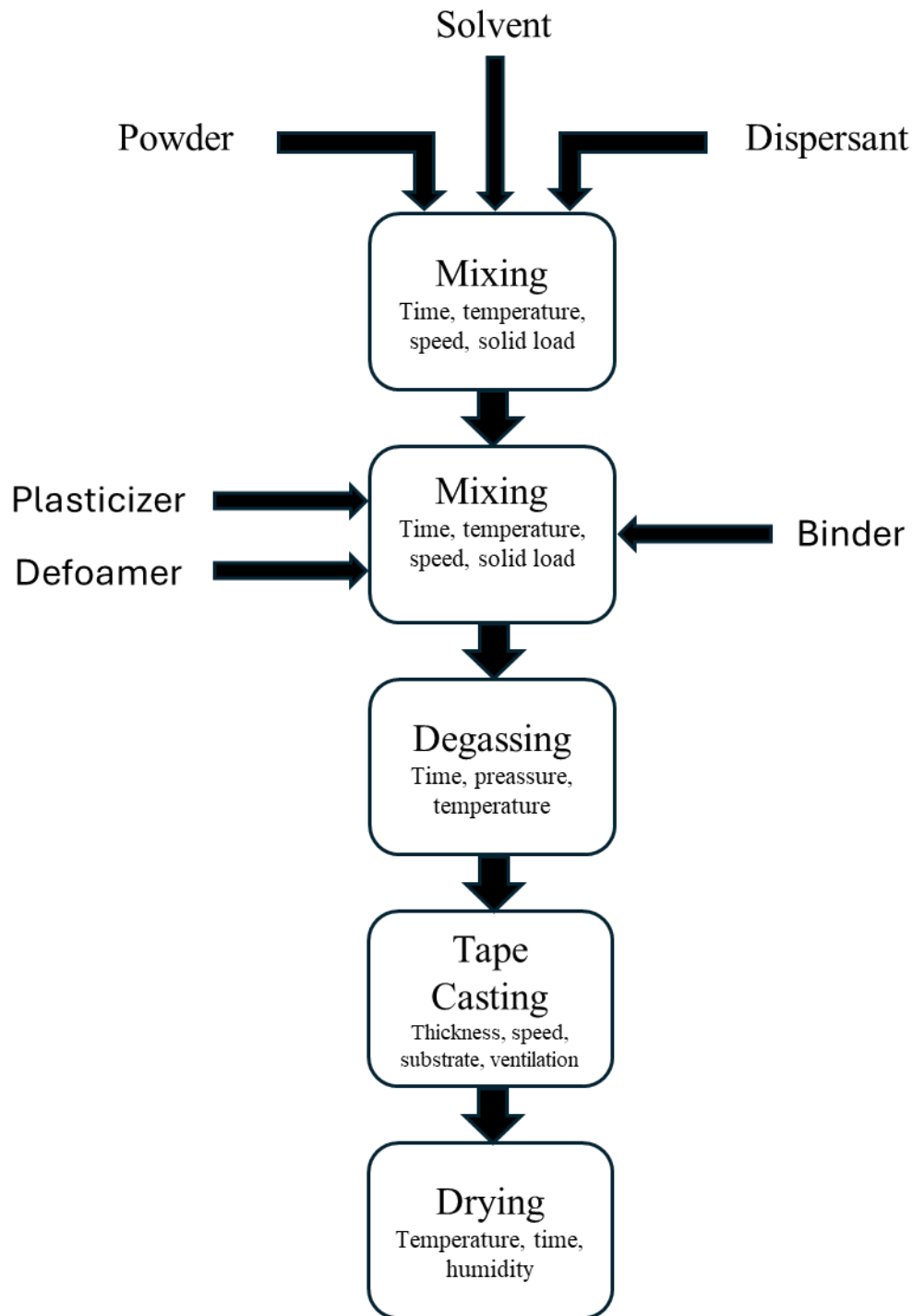


Figure 3-2 Example production flowsheet for a tape casting process of a MCFC matrix. In each step some of the main parameters that could have an effect on the outcome have been stated.

Table 3-1 Reassuring table of the main recipe found in literature for MCFC matrix production

Solvent	Binder	Plasticizer	Dispersant	Defoamer	Additives	Milling Parameters	Reference
Cyclohexanone/Butyl Alcohol (1:1)	PVB	Polyethylene Glycol	Triolein	Silicone Oil	Al ₂ O ₃ fibers (0.2 wt%)	Ball mill: 10 h	[75]
Ethanol	PVB	Dibutyl Phthalate	Solsperse 20000	Agitan DF300 M	None	Planetary ball mill: 18 h	[73]
Ethanol	PVB	Dibutyl Phthalate	Not specified	Not specified	MnO ₂ , TiO ₂	Attrition milling parameters not specified	[76]
Ethanol/Toluene	PVB	Dibutyl Phthalate	BYK - 110	SN D-348	None	Ball mill: 96h	[72]
Ethanol/Iso propanol	PVB	Polyethylene Glycol	BYK - 110	Not specified	Alluminum based fibers	Ball mill: 22h	[77]

3.3 Electrodes

In MCFCs, the electrodes allow the electrochemical reactions that drive power generation to happen. The anode is responsible for hydrogen oxidation, while the cathode reduces oxygen and carbon dioxide to form carbonate ions. These ions migrate through the molten carbonate electrolyte, completing the ionic circuit [70].

Due to the high operational temperature of MCFCs ($\sim 650^\circ\text{C}$), electrode materials must exhibit [78]:

- Chemical stability in the molten carbonate environment.
- Thermal and mechanical durability.
- High catalytic activity toward the respective reactions.

3.3.1 Electrode Materials

- Anode:

Nickel based plates, such as Ni/10% Cr and Ni/5% Al alloys, are commonly used as anode materials in MCFCs. Adding chromium or aluminium enhances sintering resistance and structural stability at high operational temperatures ($\sim 650^\circ\text{C}$). These alloying elements facilitate the formation of compounds like LiCrO_2 and LiAlO_2 at grain boundaries, which improve creep resistance and prevent sintering of the anode during operation [79], [80].

- Cathode:

Lithium-doped nickel oxide (LiNiO_2) or Nickel Oxide (NiO) is widely used. Li-doping helps stabilize the NiO structure and mitigates solubility issues in the molten carbonate, which would otherwise lead to degradation over time [81].

3.3.2 Physical Characteristics

Two critical factors influence the performance of electrodes:

- Porosity: it is required to allow for the dual function of gas diffusion and electrolyte adsorption, the optimal range between anode and cathode is slightly different, it's around 55% for the anode [82] while for the cathode a higher porosity is necessary. This is because the cathode is oxidised in situ, and during this process, the porosity decreases. The optimal starting porosity for the cathode is around 60 – 65% [83].
- Pore Size: a similar concept to the porosity goes for the pore sizes, the anode was determined to have an optimal pore size between 3 to 6 μm [84]. For the cathode on the other hand, being that during oxidation these pores tend to close, the pore size optimum is higher, around 6 to 12 μm [83].

3.3.3 Performance-Limiting Factors in MCFC Electrodes

- Anode:

The anode encounters distinct degradation mechanisms. Primarily, the high-temperature operating conditions can induce sintering, leading to the coalescence of nickel particles and the progressive loss of the porous structure required for effective operation. Concurrently, the combination of elevated temperatures and pressure gradients can drive particle migration and grain boundary movement, resulting in creep formation within the anode. This formation may lead to gas leakage or electrolyte loss, compromising cell performance. These adverse effects can be mitigated through the incorporation of suitable additives such as aluminium (Al), chromium (Cr), copper (Cu), or titanium (Ti), which help stabilize the microstructure and enhance mechanical integrity [84], [85], [86], [87].

- Cathode:

Over time, the cathode degrades via an acid mechanism, resulting in the formation of degradation products that subsequently deposit within the electrolyte matrix [88]:



A significant portion of research in cathode development focuses on identifying innovative materials capable of mitigating this effect. Among the proposed strategies, the incorporation of cobalt or the lithiation of cathode materials have shown potential; however, these approaches often result in a decrease in electrical conductivity [89], [90]. This phenomenon represents one of the most critical limiting factors affecting the long-term operational durability of molten carbonate fuel cells (MCFCs) [91].

3.3.4 Fabrication

Regarding fabrication, the process closely resembles that used for the electrolyte matrix, typically involving ball milling followed by tape casting. The primary distinction lies in the requirement for a sintering step prior to integrating the electrode into the cell, as can be seen in Figure 3-3. Various sintering protocols have been proposed, aiming to optimize both the duration and temperature of the process to enhance electrode performance and structural stability. Additionally, the atmosphere under which sintering occurs, commonly a reducing environment, is also under investigation, with alternative atmospheric compositions being explored to further improve material properties and overall cell efficiency. The main literature recipes can be found in Table 3-2 and Table 3-3.

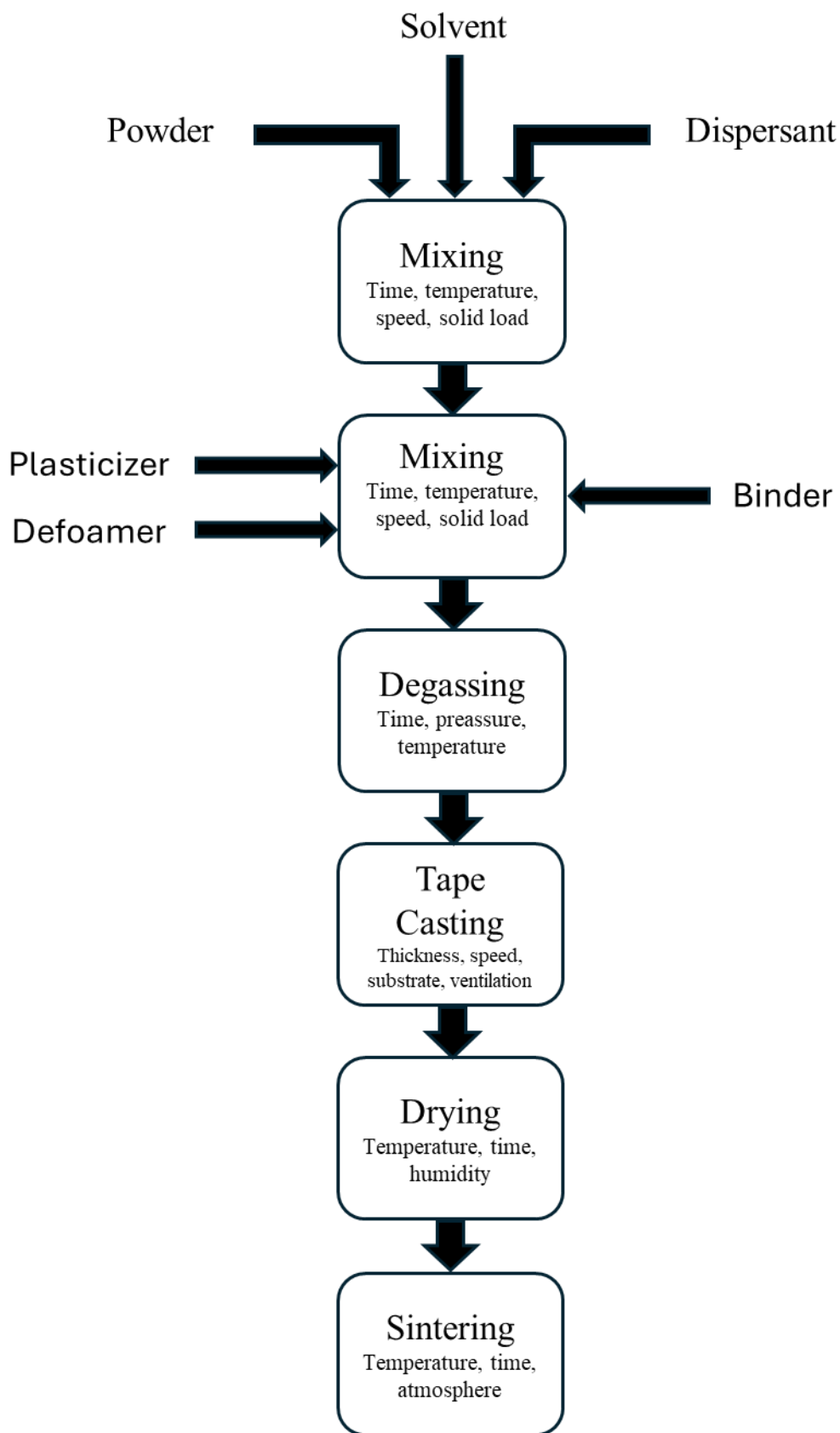


Figure 3-3 Example production flowsheet for a tape casting process of a MCFC electrode. In each step some of the main parameters that could have an effect on the outcome have been stated.

Table 3-2 Main literature recipes for MCFC cathode production

Solvent	Binder	Plasticizer	Dispersant	Additives	Starting powder	Milling Parameters	Sintering Conditions	Reference
Cyclohexanone/butyl alcohol (CHN/BA)	PVB	PEG	Glycerol trioleate	Not specified	Carbonyl nickel	2h + 4h in Ball Milling	Not specified	[92]
Cyclohexanone/butyl alcohol (CHN/BA)	PVB	PEG	Not specified	Rare earth oxide powder (CeO ₂ : 70.35%, La ₂ O ₃ : 13.83%, Pr ₂ O ₃ : 3.59%, Nd ₂ O ₃ : 12.23%)	Carbonyl nickel	4h + 4h in Ball Milling	25 to 200°C (1°C/min) – at 200°C for 2 h – (1°C/min) – 400°C for 4h – (2°C/min) – 500°C for 2h – (2°C/min) – 850°C for 6h – (-1°C/min) (75% H ₂ , 25% N ₂)	[87]
Distilled water	Carboxymethyl cellulose and Hydroxypropyl methylcellulose	PEG + Glycerine	-	Silver, Starch and polyvinyl butyral	Carbonyl nickel	-	2h at 200°C, 2h at 400°C, 1h at 800°C (5% H ₂ , 95% N ₂)	[93]
Ethanol and toluene	PVB	Dibutyl Phthalate	Not specified	-	Co/Ce coated Nickel powder	24h + 5h in Ball milling	25°C to 750°C/850°C/950°C (3°C/min)	[94]
Cyclohexanone/butyl alcohol (CHN/BA)	PVB	PEG	Glycerol trioleate	ZnO powder	Carbonyl nickel	4h + 4h in Ball Milling	850°C for 1h (75% H ₂ , 25% N ₂)	[95]
Xylene/Ethanol	PVB	Butylbenyl Phtalate	Fish Oil	-	Carbonyl nickel	4h + 24h in Ball Milling	-	[96]

Table 3-3 Main literature recipes for MCFC anode production

Solvent	Binder	Plasticizer	Dispersant	Additives	Starting powder	Milling Parameters	Sintering Conditions	Reference
Ethanol/toluene	PVB	PEG	BYK - 110		NiAl (5wt%) + Ti (3 – 5wt%)	24h + 48h in Ball Milling	650°C for 2h in reducing atmosphere	[97]
Not specified	Not specified	Not specified	Not specified -	3% stearic acid	35% Ni - 15% Cr - 50% Cu	-	950°C for 2h in reducing atmosphere	[98]
Ethanol/toluene	PVB	PEG	BYK - 110		NiAl (5wt%)	24h + 48h in Ball Milling	950°C for 1h in reducing atmosphere (10%H ₂ , 90%N ₂)	[99]
Not specified	Not specified	Not specified	Not specified	-	Ni – 10wt% Cr	-	1000°C for 30 min in reducing atmosphere	[100]
Ethanol	PVB	Polyethylene Glycol	Glycerol	-	Ni	Ball mill: 48 h	800°C with CO ₂ and O ₂	[101]

3.4 Electrolyte

The electrolyte in MCFCs is composed consisting of a molten mixture of alkali metal carbonates, most commonly lithium carbonate (Li_2CO_3) blended with either sodium carbonate (Na_2CO_3) or potassium carbonate (K_2CO_3), to form a eutectic composition that lowers the melting point and improves ionic conductivity. [102], this is seen in Table 3-4.

Table 3-4 Melting points of pure salts and the main eutectic salt compositions used in MCFC applications [103].

Salts	Melting point [°C]
Pure Li_2CO_3	723
Pure Na_2CO_3	854
Pure K_2CO_3	891
$\text{Li}_2\text{CO}_3 - \text{K}_2\text{CO}_3$ (62–38 mol%)	498
$\text{Li}_2\text{CO}_3 - \text{Na}_2\text{CO}_3$ (52–48 mol%)	501

This electrolyte is the heart of the fuel cell, as it allows the formation of the carbonate CO_3^{2-} , which is responsible for the ionic conductivity inside the cell.

The main issues with the electrolyte are two-fold: one is its corrosive properties, and on the other hand, evaporation. The degradation of the NiO cathode inside the strongly corrosive electrolyte is one of the reasons that can cause a short circuit inside the matrix, as the corroded nickel can deposit inside the matrix layer and in extreme cases cause the short circuit of the two electrode compartments [104]. Evaporation rates are affected by operating temperature, electrolyte composition, and system pressure, and while optimisation can be done through optimisation of the conditions, the evaporation is still a critical life-limiting factor for the cell [104].

Comparing the two main choices of electrolyte that are being used, $\text{Li}_2\text{CO}_3 - \text{K}_2\text{CO}_3$ (62–38 mol%) has an ionic conductivity of 1.31 S cm^{-1} compared to the conductivity of $\text{Li}_2\text{CO}_3 - \text{Na}_2\text{CO}_3$ (52–48 mol%) that reaches 2.06 S cm^{-1} , meaning that the second one has a higher performance [105], [106].

However, the $\text{Li}_2\text{CO}_3 - \text{K}_2\text{CO}_3$ eutectic has a higher dissolved O_2 at 650°C at $1.7 \times 10^{-1} \text{ mol L}^{-1} \text{ atm}^{-1}$ compared to $1.1 \times 10^{-1} \text{ mol L}^{-1} \text{ atm}^{-1}$ for $\text{Li}_2\text{CO}_3 - \text{Na}_2\text{CO}_3$ (52–48 mol%) at 650°C [107]. This allows it to have a better performance initially, but suffering for long term [106].

For lab scale where component testing is interesting, using $\text{Li}_2\text{CO}_3 - \text{K}_2\text{CO}_3$ can be a good compromise to optimize time, and has been used in the testing phases for this thesis.

4 Experimental production and testing of materials

4.1 Lab set up

At the beginning of 2023, a new laboratory was established with the specific objective of advancing research on MCFCs for CCS applications. This initiative, named Caplab, was the result of a collaborative effort between the University of Genoa and the industrial partner Ecospray Technologies Srl. Since its opening, the laboratory has undergone significant expansion, both in terms of equipment for material synthesis and cell testing, as well as in personnel, including researchers and students who have actively contributed to the development of new components while gaining valuable research insight. This synergistic and multidisciplinary approach has developed a dynamic research environment, enabling steady progress in the field.

During the PhD period, Caplab progressed through different development stages, with laboratory capabilities expanding as additional equipment became available. Consequently, the experimental activities reported in this thesis reflect the instrumentation accessible at the time each test was performed. Unless otherwise stated, the experimental campaign presented in this work, including the definition of the test matrix and operating windows, as well as fabrication, characterisation and electrochemical testing, was carried out by the author in collaboration with the research group and supporting MSc and BSc students. The instruments most relevant to this work are listed below.

- Cell station 1:

This custom-built cell testing station enables precise and flexible gas flow management to the fuel cell using multiple electronically controlled flowmeters. Humidification of the gases is achieved through the usage of two dedicated humidifiers, one for each electrode. While most gases were supplied via gas cylinders located on the laboratory roof, hydrogen was generated in situ using an AEM electrolyser, primarily for safety considerations. At the core of the setup is a furnace managed by PLC, allowing for precise temperature regulation, as can be seen in Figure 4-1. Temperature monitoring is implemented not only within the furnace but also within the cell itself, facilitated by thermocouples integrated into the cell frame. The cell frame has undergone multiple design iterations, exploring various geometries and dimensions to optimize performance and reliability. Later, the AEM electrolyser has been substituted with a smaller Proton Exchange Membrane (PEM) electrolyser because of reliability issues.



Figure 4-1 These are the main components of cell station 1. a) This section represents the central part of the setup. The furnace is located at the centre and houses the cell, which is inserted together with its cell frame. Gas lines from the flowmeters are connected to the cell from both the left and right sides. The two cylinders on both sides are the humidifiers. b) An AEM electrolyser, which provides hydrogen to cell station 1. c) The cylinders on the roof were initially both responsible for CO_2 and N_2 gases, successively only the CO_2 tanks were kept.

- Ball miller:

Ball milling, previously discussed in the literature review of cell component fabrication, has been identified as one of the most widely adopted techniques for the homogenization of component slurries. The ball milling equipment available in our laboratory is compatible with a range of vessel sizes; however, 250 mL containers were predominantly utilized for our purposes, as can be seen in the operating setup in Figure 4-2. The system allows for the simultaneous processing of up to six vessels, though over time this limitation has emerged as a bottleneck in the overall production workflow, particularly when scaling up material production.



Figure 4-2 Ball miller with six 250 ml vessels being mixed on it.

- Gas Chromatograph:

The gas chromatograph (GC) serves as a valuable analytical tool for monitoring the processes occurring within the fuel cell. Gas chromatography enables precise determination of the composition of the exhaust gases, providing critical insights into the cell's operational behaviour [108], primarily by giving an indication on how much CO_2 has migrated between the two cell electrodes. However, due to the challenging conditions at the cell outlet, including high humidity and the potential formation of carbon deposits, direct sampling poses a risk to the instrument. To mitigate these risks, the gas stream first passes through a heated line to prevent condensation, followed by a condensation unit that cools

the gas and facilitates the removal of water. This pre-conditioning ensures the gas is in a suitable state for accurate and safe GC analysis, the whole setup can be seen in Figure 4-3.



Figure 4-3 The GC setup is arranged on a two-tier tray. On the lower level, a condensation unit is installed to remove water vapour from the gas stream prior to analysis. On the right-hand side, a high-purity helium cylinder is provided as the carrier gas required by the GC and to maintain the appropriate backpressure. The upper level hosts the GC instrument together with the associated control unit and computer, which are used for instrument operation and data acquisition/visualisation.

- Tape caster:

The tape caster, that is intrinsically connected with component production, allowed us to control the thickness and spread of our components. This instrument seen in Figure 4-4, often also used in the textile industry, uses a variable height blade with two side control and a stretched sheet, typically Mylar which is a very smooth plastic, on which the slurry is deposited and spread. Using the blade the slurry is dragged uniformly across the sheet. Both the viscosity of the slurry but also the material of the sheet can have a significant impact on the casting process.



Figure 4-4 Tape caster; on top the black casting blade, on the sides the two height regulations can be seen, with their reading instruments. In the middle, under the blade the casting sheet should be stretched.

- Voltmeter:

An important aspect of cell testing is the continuous evaluation of the cell's electrical potential, which provides essential information regarding its performance and operational state. By monitoring the

voltage and current output, it is possible to assess gas utilization efficiency, determine power output, and identify deviations from expected behaviour. Furthermore, advanced electrochemical techniques such as Electrochemical Impedance Spectroscopy (EIS) allow for a more detailed characterization of the cell's internal mechanisms. These analyses can reveal internal resistances, mass transport limitations, and kinetic bottlenecks, thereby identifying critical limiting factors within the cell, that can give important suggestions toward component optimisation. The two components of the voltmeter can be seen in Figure 4-5, whereas the unit above is the instrument for low current ranges, while the lower instrument can be used in combination with the first to increase the operative range.



Figure 4-5 Voltmeter on top, that is connected to a PC for the reading, on bottom a booster module is attached, this is because the normal voltmeter is limited to a range of $\pm 6V$ and $\pm 2A$, while the booster allows to reach $\pm 40V$ and $\pm 20A$.

In the subsequent months and years, additional instruments were acquired to support and enhance the growing expertise in the specialized areas of component fabrication and fuel cell testing.

- Cell station 2:

The testing procedures conducted on Cell Station 1, which will be discussed in detail later, revealed several critical factors that could influence cell performance. Cell Station 1 was progressively refined over time, with iterative improvements implemented after each test cycle based on experiential feedback. In parallel, a second cell station was developed as seen in Figure 4-6, incorporating the foundational principles of the first system, particularly its PLC-based control architecture, while integrating enhancements informed by the operational limitations identified in Cell Station 1. Notably, significant advancements were made in the design of the humidification system; unlike the basic saturation-based units used in the first station, The new humidifiers are based on a more advanced operating principle. While the previous design relied on gas saturation by bubbling the stream through heated water at a controlled temperature, the new units humidify the flow by directly injecting (spraying) water into the gas stream. Furthermore, a dedicated electrolyser was acquired for cell station 2, and the electrolyser of cell station 1 was changed, as the first one that was used incurred in stalling issues.

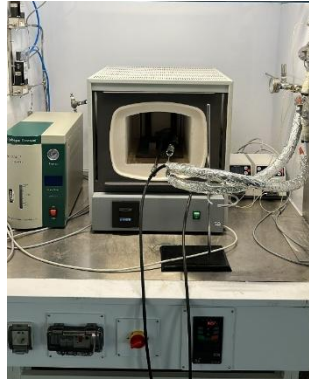


Figure 4-6 Cell station 2: as seen in cell station 1, the hearth is a furnace, but in this case the feed is from the right side for both electrodes, this is to make space for a dedicated electrolyser on the left side of the cell. The humidifiers are attached to the right side of the hood walls. Critically, to avoid condensation of the steam before entering the cell two heating cables are used.

- Nitrogen generator:

The nitrogen generator is based on an air separation unit (ASU) as seen in Figure 4-7, which separates nitrogen from oxygen in ambient air using a combination of pressure and membrane technology [109]. To ensure reliable operation, the system includes a refrigeration unit to remove moisture from the air stream, as humidity can lead to membrane clogging and reduced efficiency. The implementation of the nitrogen generator eliminated the dependence on nitrogen gas cylinders, which were associated with various logistical challenges and frequently led to delays in cell testing.



Figure 4-7 Nitrogen generator; on the left side the gas enters, the two gauges show firstly the input pressure of the air and the second one for the output pressure of the nitrogen.

- Mercury porosimeter:

A critical part of component production is to check on their main characteristics, amongst which the porosity and pore size distribution are the most important, both for the matrix but also the electrodes. The acquisition of a mercury porosimeter was therefore of upmost importance. This device, as seen in Figure 4-8, can provide a detailed and global view of the component characteristics, utilising mercury as a non-wetting liquid [110]. The complexity of the instrument also required a long adaptation period, but some of the obtained results were useful to determine the correct development path for the materials. The device houses two different pressure operating units. The low-pressure unit, housed behind the blue doors on the right side of the device, enables simultaneous testing of up to two samples. In this mode, mercury is intruded into the porous structure of the sample under vacuum conditions,

allowing for mercury intrusion inside the component and testing of larger pores and structures. For finer porosity characterization, the high-pressure module is employed, located in the piston assembly at the top of the instrument. The low-pressure mode is generally effective for measuring pores down to approximately 1 micron in diameter. However, for the detection of nanopores and more refined structural analysis, the application of high pressure becomes necessary. This dual-mode capability is particularly important in the context of MCFC component development, where accurate characterization of porosity across a wide size range is crucial. Since the targeted pore sizes in matrixes approach the 1-micron threshold, both measurement regimes are required to ensure comprehensive porosity profiling.



Figure 4-8 The mercury intrusion porosimeter, depicted in the accompanying figure, is equipped with two distinct testing modules to accommodate a broad range of pore size analysis.

- Automatic tape caster:

The tape caster that was available when the laboratory opened was enough to start material production and testing, but had several drawbacks, stemming from the non-replicability of many of the variables that were involved in the process, being for example the speed the blade is dragged above the tape or the evaporation temperature of the sheet. The new tape caster, as seen in Figure 4-9, on the other hand provided the possibility to control the process speed, blade height and the temperature of the sheet the slurry was applied on.



Figure 4-9 The above depicted tape caster is automatic, using motors to move the sheet at a determined speed and can provide heating from below to control the evaporation speed. As can be seen comparing it to the manual tape caster the dimension is much more like an industrial scale.

- Infrared gas analyser (IR-Spectroscopy):

The IR allows for a fast gas analysis of a gas composition that has previously been calibrated, utilising the specific infrared adsorption of each component [111]. The IR module was calibrated for the IR-active species (CH_4 , CO and CO_2). H_2 and O_2 were quantified using the analyser's non-IR Thermal Conductivity Detector (TCD), while N_2 was obtained as balance where applicable. To do this many tests were made, varying the gas compositions using the electronic flowmeters. After that, the IR can check the gas output of the cell continuously. The IR analyser and GC were used in a complementary manner. The GC provides higher analytical robustness because it separates the gas mixture into individual components prior to detection, thereby reducing cross-sensitivities and enabling a wider range of compositions to be quantified with good selectivity. In addition, GC quantification typically offers a lower detection limit and a broader linear dynamic range than IR-based measurements, and it is less constrained by narrow calibration windows for each species. Conversely, the IR analyser offers continuous, real-time monitoring of the main IR-active species, which is not achievable with the GC due to its batch-sampling nature and longer analysis time per injection. For this reason, the IR was used for continuous process control (trend monitoring), while the GC was used for accurate, flexible composition verification and periodic calibration checks.



Figure 4-10 The IR - Spectroscopy in picture has both a small interface on the instrument itself and one that can be remotely accessed through ethernet connection. Importantly, the same rig as for the GC is used to clean the gases as also this instrument requires dry gases to avoid ruining the sensors.

- Controlled atmosphere oven:

Importantly, sintering requires both high temperatures, often above 800 °C, and controlled atmospheres to prevent oxidation of metallic constituents. This was impossible with the ovens that were available for the cell stations, as the highest temperature that could be reached was exactly 800°C. Therefore, another oven was acquired as seen in Figure 4-11, with the possibility to be programmed electronically, have a continuous gas flow and reach temperatures of up to 1200°C. This allowed to start sintering processes on the green electrode tapes.



Figure 4-11 Controlled atmosphere oven; the external oven structure can reach up to 1200°C, while a reinforced chamber is inserted inside to allow for the formation of the controlled atmosphere.

- Caplab Dashboard personalised management software:

In collaboration with a student from informatics who was performing his dissertation at the Caplab, a software was developed that was tailored to the needs of the lab personnel. The aim was to develop an environment that could allow optimise both the workflow inside the lab but also the data analysis done later. The main features as seen in Figure 4-12 are:

- Inventory: This inventory related compounds through QR codes. It is possible to change material quantities, add a safety card and add remarks like the storage location.
- Data storage: The dashboard was projected in a way that it could grow with the growing needs of the lab. This was done by making personal tabs possible, inside which files could be saved. For each file a few short comments could then be visualized to have a fast overview.

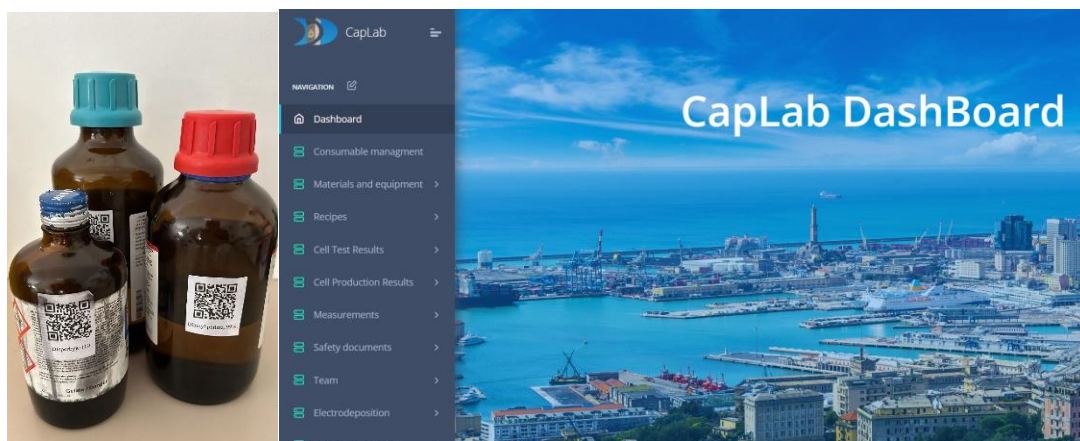


Figure 4-12 On the left an image of the QR codes applied to different liquids used in the lab, on the right the main page of the dashboard.

All these instruments were vital in the work that will be presented inside the next chapter, but the timeline of provision of the instruments is also necessary to allow for a deeper understanding of the choices that have been made.

4.2 Components

After the literature review, three recurring gaps were identified. First, the MCFC materials literature remains relatively limited and is still largely anchored to a set of foundational studies, many of which date back to the early 2000s, while more recent contributions frequently build upon established formulations and operating concepts, indicating clear opportunities for further optimisation and modernisation of both materials and manufacturing routes. Second, a significant fraction of published experimental work is performed at laboratory scale which is highly valuable for component screening but provides less direct insight into manufacturing repeatability, component handling, and scale-up constraints. Third, although the literature often identifies the main classes of raw materials employed, key information on the specific chemical identities, grades, purities, and processing conditions is frequently incomplete or omitted (as seen by the amount of “not specified” present in Table 3-1, Table 3-2 and Table 3-3). This lack of methodological transparency hampers reproducibility and complicates technology transfer to new laboratories, which consequently requires extensive preliminary trials to establish robust composition ranges and processing protocols.

4.2.1 Matrix

The matrix is a critical component for the molten carbonate fuel cell, because of its specific structural requirements for the fuel cell operation. As discussed, the way to achieve this is to reach a high porosity with small pore size ($\sim 50\%$ porosity and pore size $< 1\ \mu\text{m}$) that allow, together with the molten carbonate, to form an optimal dual effect of gas separation and ionic transport.

Within the scope of this thesis, a matrix was to be produced, using if possible less expensive and toxic components with comparable performance to the once found in literature, and with a production process that could have a good scale up potential.

A total of more than 170 different matrix batches has been made, with differing degrees of success. It must be remembered that the research started with no real indication on the component amounts for the starting batches, if not some incomplete indications that were rarely available.

Through a first check of the materials that were available in the lab, the first recipe to test was determined to be the recipe from the Korean Institute of Science and Technology (KIST) [72]. By discussion with other research centres an idea of reasonable weight percentages was determined and the recipe described in Table 4-1 was tested.

Table 4-1 Matrix recipe based on the KIST literature formulation, with weight fractions estimated from fragmented literature information and formulation rationale (meaning enough to ensure sufficient solvent to accommodate the solid loading and achieve a castable slurry).

<i>Role in the mixture</i>	Compound	Reasonable weight distribution:
<i>Base powder</i>	γ -LiAlO ₂	36 %
<i>Solvent 1</i>	Ethanol	14 %
<i>Solvent 2</i>	Toluene	33 %
<i>Dispersant</i>	BYK – 110	1 %
<i>Binder</i>	Polyvinyl Butyral (Butvar B-98)	9 %
<i>Plasticizer</i>	Dibutyl Phthalate	6 %
<i>Defoamer</i>	SN D-348	1 %

The initially proposed ball-milling time was 96 h; however, the literature review indicated that this duration should be distributed across multiple milling steps rather than mixing all components in a single stage, so it was chosen to first mix the solvents toluene and ethanol together with the powders and dispersant, and in a second step the remaining compounds have been added. After the 96h milling time, the mixture was cast, and the casting was put to dry under a hood to avoid safety risk connected with solvent evaporation.



Figure 4-13 First matrix test at the Caplab laboratory following literature recipes.

While it appears evident from Figure 4-13 how the obtained results did not reflect the overall desired result of a homogeneous surface, it was the beginning for matrix testing at the Caplab. The main take aways were the following:

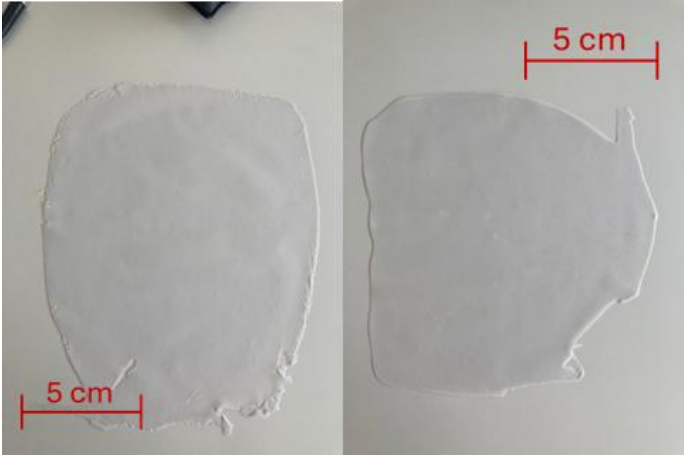
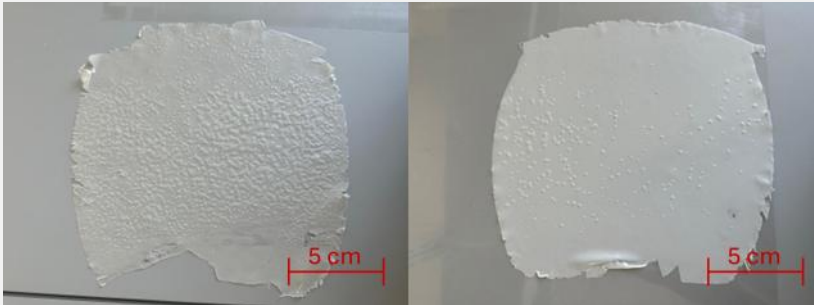
- An optimisation of the mixing times was required to allow for better powder dispersion inside the slurry, as it can be seen how there are still some solid agglomerates.
- Many bubbles were still present inside the casted material, suggesting the need for a better degassing step.
- The thickness of the sheet was not homogeneous, suggesting a need to optimise the way the substrate of the casting is fixed to the tape caster.

To simulate the characteristics that the matrix will have once it is put inside the cell and brought to working temperature, a sintering process is done, which consists in heating the matrix to 650°C outside the cell. This process allows all the organic compounds to be burned out, leaving only the ceramic matrix behind. Doing so the obtained result shows the porosity that the matrix will have at its operating conditions.

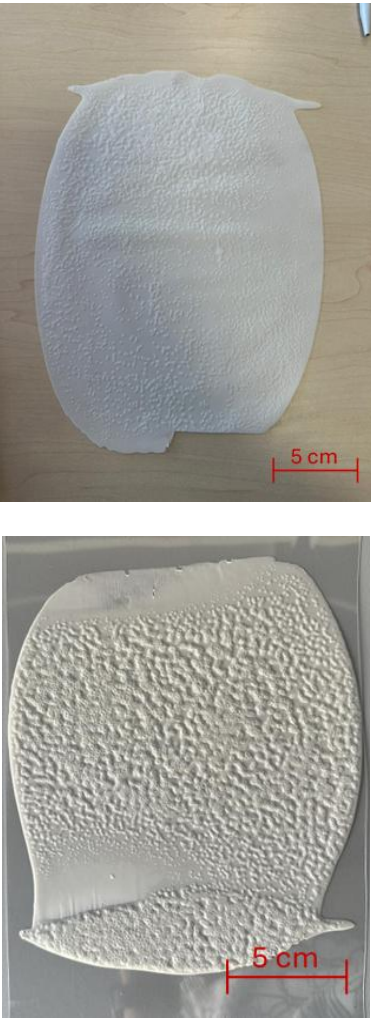
Starting with these observation, different tests were done, each with the aim of tackling systematically one of the above-mentioned issues. In the following Table 4-2, the matrix number, its recipe blueprint and the differences to the one discussed above are discussed.

Table 4-2 Experimental campaign matrix production May - September 2023

<i>Number</i>	Differences and considerations	Image
2	• Increase of vacuum time and pressure. • The degassing caused a phase separation; while removing the bubble is important, exceeding can cause issues on its own.	
3 - 4	• Decreases vacuum time, but vessel put inside a hot water bath (40°C) to avoid desiccation. • The results looked more promising, although the homogeneity of the cast was still not achieved. The sintered layer was very brittle.	

<i>Number</i>	Differences and considerations	Image
5 - 6	- To increase the stability of the matrix, a percentage of alumina has been inserted inside the powder mixture [75] (9.4wt% in 5 picture on the left, 18,8wt% in 6 picture on the right). - After the sintering process, the matrix 5 is significantly less brittle than the matrix 6 and the matrix 4, suggesting that adding a small amount of alumina could help the stability of the ceramic substrate.	
7 - 8	- To increase the understanding of the effect of the alumina on the matrix, different alumina contents have been tested (4.5wt% in matrix 7 picture on top, and 28.8wt% in matrix 8 picture on the right). - The obtained sintered materials were still very fragile, as the surfaces did not reflect the expected and reasonable effect of adding or removing alumina, but suggested issues for the drying process. This means that there	

<i>Number</i>	Differences and considerations	Image
	were still some unknown issues not considered. Furthermore, a higher degree of replicability was required in the test going on.	
9	• To supplement our initial knowledge of matrix production, a new recipe was tested, from WTU [73]. • The result had a very irregular surface and presented many wrinkles. The test was made in two separate batches, and both were identical, suggesting an issue with the recipe.	
11, 13	• Following the same logic a recipe by ParisTech was also tested out [77]. • While the smoothness of the surface was far superior to the matrix 9, the result still presented some wrinkles.	

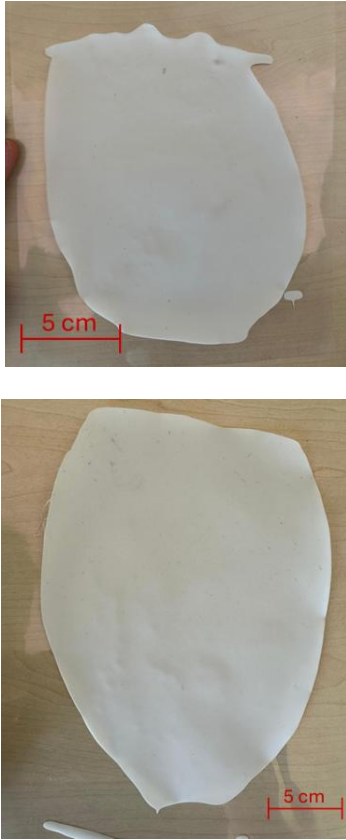
<i>Number</i>	Differences and considerations	Image
10, 12, 14 - 16	• Having seen that the KIST recipe presented the best starting point for the matrix production at the Caplab, different test for drying conditions were studied, as it was noted how the atmospheric conditions changed the drying, and the drying changed the morphology. • The main results were that while heating allowed the release of more bubbles, excessive amounts caused the solvent itself to start bubbling, making the surface far too uneven. It was determined, that while not constant, atmospheric drying had less issues than applying heat.	

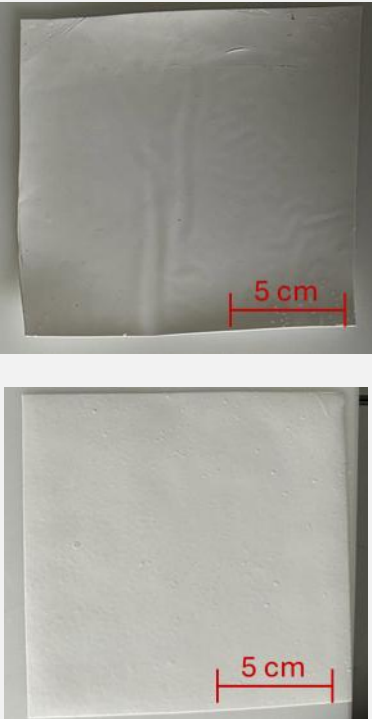
The experimental campaign was structured in two consecutive phases. The first phase focused on reproducing representative literature procedures to establish a reliable baseline and verify transferability to the available equipment and operating constraints. Once feasibility was confirmed, the second phase adopted a parameter-screening approach to identify the process variables with the largest impact on component quality and cell performance under the specific conditions of the present setup. The inspection in this first experimental phase was still done without the utilisation of specific analytical techniques but based on empirical evaluation of different parameters ranging from: slurry processability (castability and stability), defect density after casting and sintering (cracking or warping of the surface). At this stage, a detailed analytical phase was not yet applicable, as the produced sheets did not meet the minimum quality requirements for meaningful microstructural characterisation.

Among the reviewed approaches, the KIST-based formulation provided the most consistent results with respect to these criteria and was therefore selected as the reference route for further optimisation. The subsequent activity focused first on reproducing the procedure as faithfully as possible and then on implementing targeted modifications aimed at improving practicality and scale-up compatibility. Toluene was substituted due to its safety and regulatory limitations in the context of future larger-scale processing, while maintaining the functional requirements of the original solvent system [112].

As a result, the subsequent phases of the campaign pursued two parallel objectives: refining the replication of the KIST recipe and identifying a viable, less hazardous alternative to toluene for matrix fabrication. The results for this study can be seen in Table 4-3.

Table 4-3 Experimental campaign for perfection of matrix production following KIST literature recipe. September 2023 to January 2024.

Number	Differences and considerations	Image
20 - 25	- Following the afore mentioned aim of firstly being able to produce a matrix from recipe, more KIST matrixes were produced, keeping the materials always the same and only varying factors as milling time, material introduction order and powder quality. - The test suggested that: a milling time of 24 h + 24 h showed good results; adding all liquids together with the solvents and the lithium aluminate powder in the first step, and only in the second one the binder and plasticizer optimised the milling process; a fine filtered powder showed more promise, as it reduced the production of agglomerates. The images on the right refer to the best obtained samples and show a significant improvement to the once from the first campaign.	

<i>Number</i>	Differences and considerations	Image
26 – 30	- Until now the used milling vessels were made of Polyethylene (PE), these were fine for the milling but because of the sticky nature of the substrate used vessels were almost always one time use. For this reason, glass vessels were chosen going forward. This change also required a consideration on the volumes that could be reasonably used for any given experiment. Furthermore, the amount of zirconia balls also depended on the volume, by the ball milling rule of 1/3 of empty volume, 1/3 of material and 1/3 of zirconia balls [113]. - It was determined that having a volume of more than 100 ml of liquids caused the loss of a lot of material during the filtering phase. The increased volume had more difficulties when it came to homogenisation and was therefore much thicker. Therefore, a volume of 250 ml vessels with a slurry load of 100 ml was kept and chosen going on.	

After the testing campaign was concluded, a significant number of matrixes based on the KIST recipe was obtained. The first campaign yielded promising results but had no component that warranted a more specific analysis, as they were all still far from the literature target. This second campaign however was analysed utilising SEM imaging, that was provided by the Electrochemistry and Corrosion Group, GEC, at the University of Genoa. This imaging had as target to provide inside into the microscopic structure, and therefore also pore size.

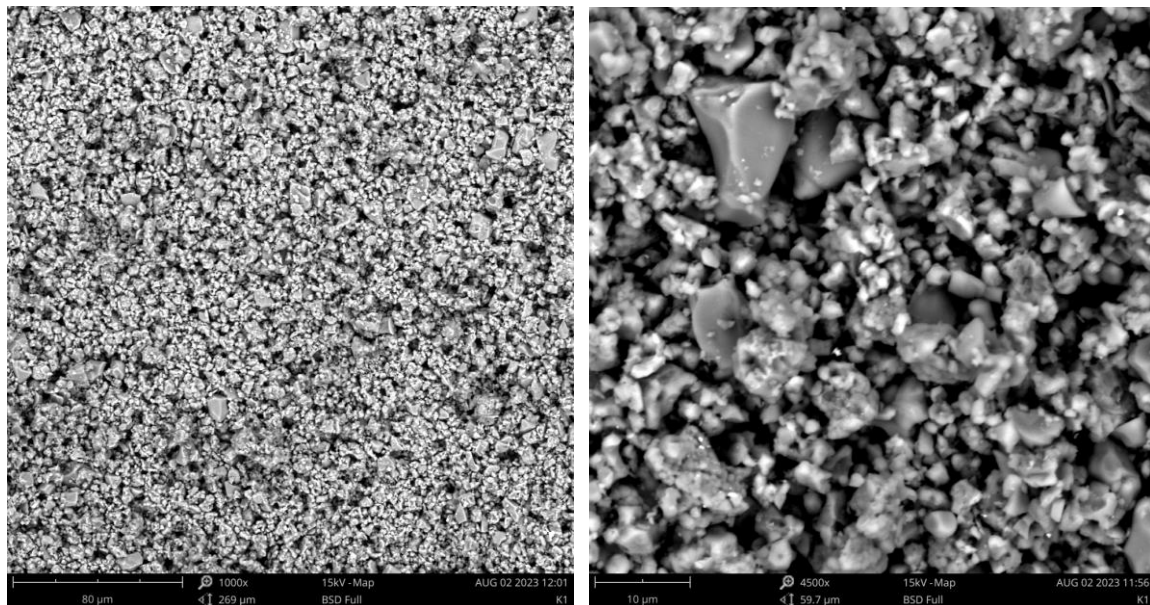


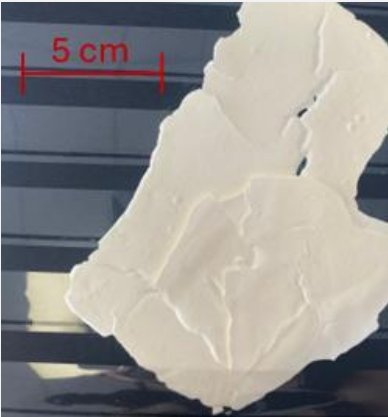
Figure 4-14 SEM imaging of a KIST recipe produced matrix by Caplab, after sintering.

From the SEM imaging in Figure 4-14 the homogeneity of the pore distribution and size can be observed. This was the first critical point that had to be checked. Secondly, enhancing the image, it was also possible to see that the average pore size was around 1 micron, which was also confirmed using an image analysis tool and applying a grey scale filter. This is also around the target dimension that was determined during the literature review. One potential issue that was determined during this analysis, was that there was a presence of some anomalies in the grain size, which although usually homogeneous presented some outliers, while still being all the same kind of chemical species. Yet, this did not seem to represent issues to the overall structural integrity of the sample.

After the analysis was done, showing highly promising results, the issue that needed solving was the removal of solvents with significant health and safety hazards from the recipe. Therefore, a new campaign was started as described in Table 4-4, although throughout some KIST recipe matrixes were still being produced to allow for cell testing to happen, which will be discussed later.

Table 4-4 Reassuring table of the main results obtained by the production of matrixes 30 to 100.

Number	Differences and considerations	Image
30 – 70	- Through research it was possible to determine that Butvar B – 98 [114] was soluble in multiple organic solvents, therefore the first test was done using an alternative green solution and removing toluene: this obviously introduced difficulties connected to the determination of the quantity of solvent, the time, the vacuum and the casting. Therefore, many different variations for all these parameters were tested - The new solvent based matrix generally showed signs of potential, resulting in a similar white tape like the one from the KIST matrix, yet after all the testing was done one thing was not solvable and it was the formation of a scaly skin layer, probably correlated to the fast evaporation of chosen solvent compared to the ethanol and toluene mixture. The images on	

	the right, coming from different batches all show this peculiarity.	
71 - 100	- Having discovered in earlier attempts that alternative solvents were viable, we found that the solvent selected evaporated too quickly. The idea was now to introduce a secondary solvent to alleviate this issue, but that still had a reduced impact when compared to toluene. - Until recipe 100, the issue of scaly skin was not completely solved, although it was alleviated.	

This experimental campaign took place for 5 months with many different tries, that ended in August 2024.

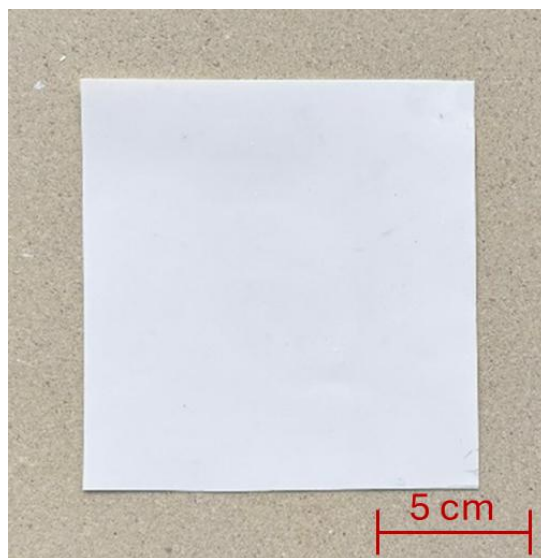


Figure 4-15 Matrix Caplab 1, that was taken to KTH and tested, giving very promising performance

The last one that was produced utilising a greener solvent mixture and was subsequently called Caplab 1 as seen in Figure 4-15. This sample was tested in Stockholm during a foreign period at the Royale Institute of Technology in Stockholm (KTH) together with sample 97. Whilst the details of the testing will have a dedicated chapter, it is noteworthy that Caplab 1 outperformed even literature results of around 120 mW/cm^2 targets, while using a non-toxic solvent mixture. This result was counterchecked by performing separate cell tests with separate batches of matrix and obtaining the same results both times. This result allowed the research to consider the obtained home-produced recipe to be working, and a characterisation of the sample was done through the newly acquired porosimeter, that showed a porosity of 60% with an average pore diameter around 0,16 micron, as seen in Figure 4-16. These characteristics indicate a matrix that is consistent with what has been described in the literature and in the dedicated chapter. Furthermore, a SEM analysis was performed to compare the result to the one obtained from the KIST recipes. Prior to performing these measurements, the matrix was sintered using the same start-up procedure adopted in the cell environment, to remove organic additives and ensure that the subsequent analyses reflect the matrix characteristics under relevant conditions.

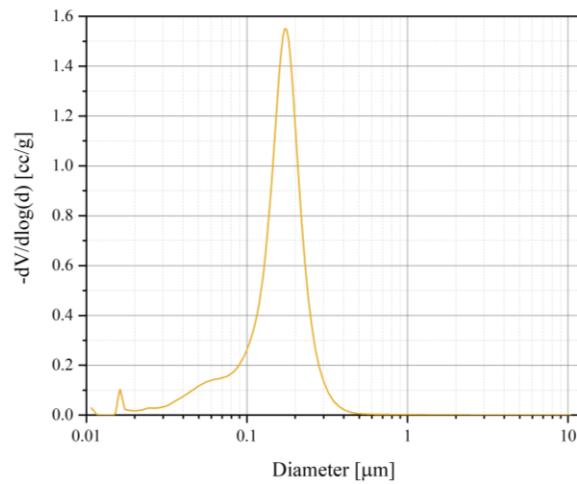


Figure 4-16 Porosimeter analysis which showed that the distribution of pores inside the sample Caplab 1 had a peak around 0,16 micron of pore size.

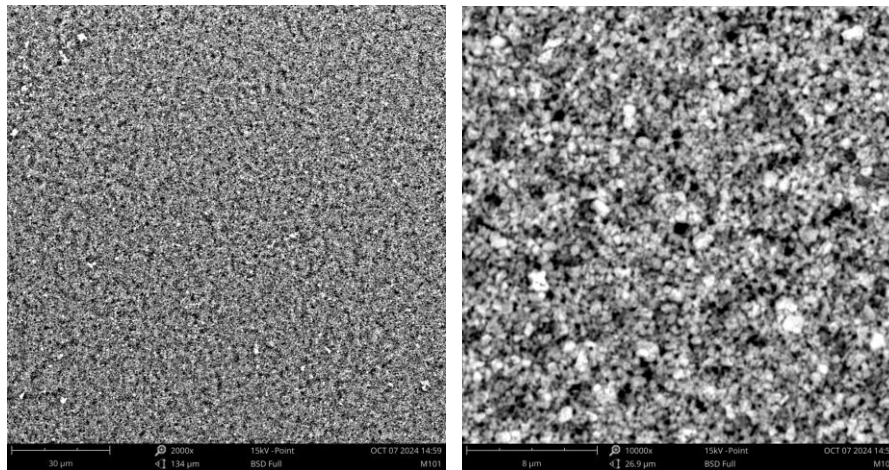


Figure 4-17 SEM images taken from the Caplab 1, left the image has a x 2000 magnification while on the right the magnification is x 10000.

From Figure 4-17 it emerges how homogeneous the distribution of pores really is, also when comparing them to the matrix produced with the KIST recipe in Figure 4-14, furthermore, the issue of bigger powder particles was solved, probably through optimisation of the milling times and zirconia ball dimensions.

After this result, the main gripes that had still to be solved were two: the long production times, as even after an optimisation, times shorter than 96h never yielded results, and the removal of DBP, Di Butyl Phthalate, which has itself safety concerns [115], like toluene before it, but is more difficult to substitute. These are still subject to studies as of the discussion of this thesis.

4.2.2 Electrodes

The electrodes in molten carbonate fuel cells are important to ensure efficient electrochemical reactions, and their structural and compositional properties are key to overall cell performance. Optimal electrodes are typically porous (~ 50% for anode, ~ 60 - 65% for cathode), allowing for effective gas diffusion, and are composed of materials that provide both high electronic conductivity and catalytic activity. The carefully engineered porosity (3 - 6 μm for anode and 6 - 12 μm for cathode) supports the triple-phase-boundary where the gas, electrolyte, and electrode material meet, thus promoting efficient charge transfer and sustaining stable operation under high-temperature conditions. This layer can only exist if the electrode is able to provide a good gas diffusion while also allowing a good interface with the electrolyte as seen in Figure 4-18.

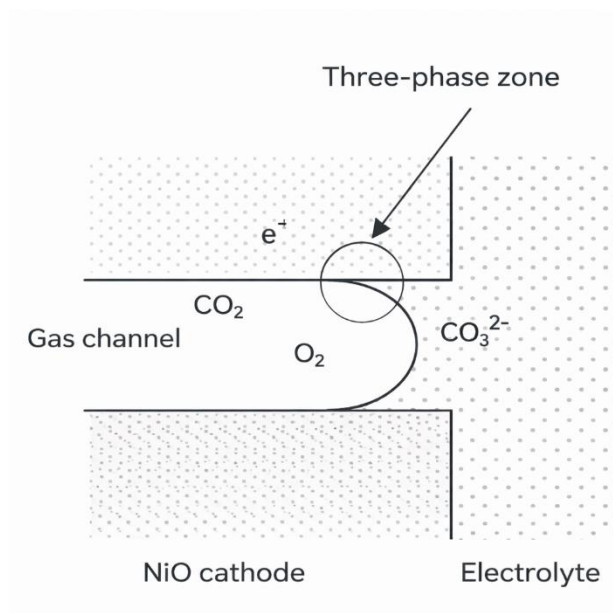


Figure 4-18 Stylised representation of the three boundary layer effect for the cathodic electrode side inside the MCFC [116]

As discussed during the chapter about the lab set up, the research into the electrodes was started later, compared to the matrix one, because it requires the utilisation of a sintering oven, that could reach temperatures around and above 800°C , which was not possible in the first year of the lab, as such an oven was not present. In the first lab expansion this oven was acquired. With this it was possible to sinter the green tapes obtained from the tape casting process.

The tape casting process as discussed during the literature review is basically the same as the one used for the matrix, with the main difference being the components used. Testing started from a completely home-made recipe, as most literature review electrodes already include compounds like Chromium [117] or Cobalt [118], which are highly toxic and were left out for the first phase of this study, while being provably useful for electrode stability. This also allowed the produced electrode to be employed either as an anode or a cathode, since in both cases the primary catalytic functionality is provided by the nickel-based phase. However, the absence of performance-enhancing additives meant that the first samples still exhibited several of the limitations highlighted in the literature review, which could be mitigated in subsequent iterations by introducing selected additives.

The initial recipe is resumed in Table 4-5 and was put together to a part of experience gained during matrix casting and a together of choices from literature, and is made for the production of a cathode ideally, even though, being that there are no additive compounds, it could be used also as an anode before the sintering process, where the porosity is mainly determined:

Table 4-5 Starting recipe for electrode production based on different literature results [92], [93].

<i>Role in the mixture</i>	Compound	Reasonable weight distribution:
<i>Base powder</i>	Ni or Ni/Al 95:5%	41 %
<i>Solvent</i>	Cyclohexane	50 %
<i>Dispersant</i>	BYK – 110	1 %
<i>Binder</i>	Butvar B-98	4 %
<i>Plasticizer</i>	PEG 400	4 %

In this case a 24h + 24h milling configuration was used, still using the same container size of 250 ml and a filling of approximately 100 ml of material, to be coherent with the matrix production. The vacuum was also done in the same way for a short period of time at a pushed vacuum. The obtained result can be seen in Figure 4-19. The homogeneity of the layer from a visual analysis suggested a good distribution of the powders and a potentially positive result.

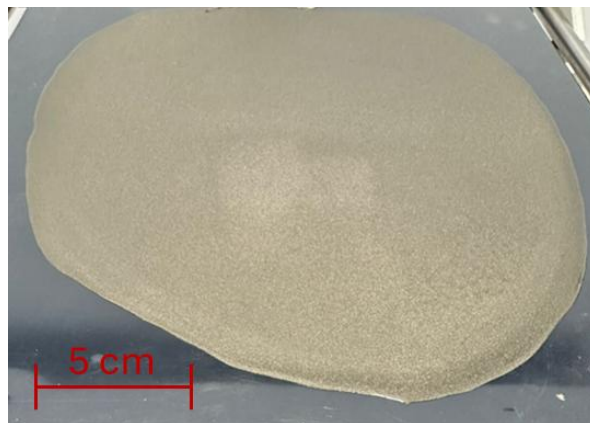


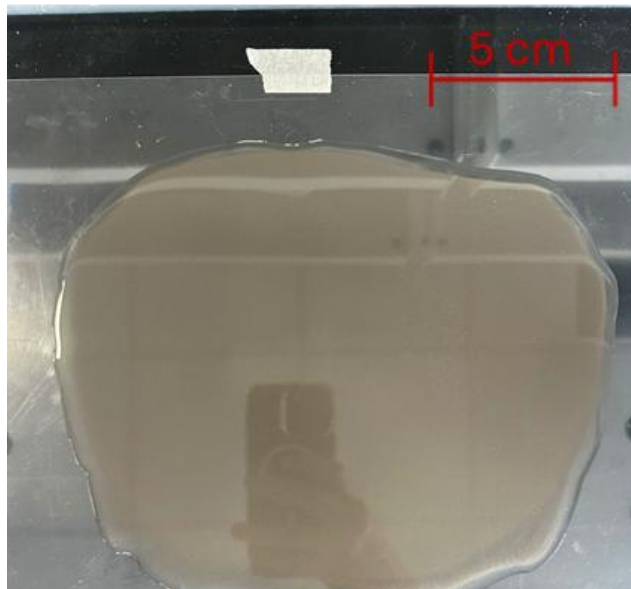
Figure 4-19 The results of the initial electrode material tests appear promising; however, the apparent quality masks thickness non-uniformities caused by the powder load, which increases lateral spreading and leads to an uneven deposited layer.

What is not conceivable in the image is the thickness of the layer, that is under 0.1 mm, making the sheet extremely thin, which can be an issue for in cell applications (where a reasonable thickness after discussion with sector experts can range between 0.3 and 0.6 mm after sintering). Furthermore, the issue was not the blade

height, but the powders inside the mixture are much heavier than LiAlO_2 ($\text{Ni} = 8.90 \text{ g/cm}^3$, $\text{LiAlO}_2 \rho = 2.62 \text{ g/cm}^3$), meaning that they tend to expand much easier and spread wider.

As with the matrix, a campaign was started as seen in Table 4-6 from this result to determine the optimal viscosity to allow the powders to stay together more and therefore the layer to become thicker.

Table 4-6 Reassuring table of the main results obtained by the production of electrodes 2 and 3.

<i>Number</i>	<i>Differences and considerations</i>	<i>Image</i>
2 - 3	• As for the matrix, the solvent system was identified as the most straightforward variable to modify. Accordingly, a solvent-screening study was carried out by testing mixtures of organic solvents to improve processability. The underlying rationale was that a slightly higher-viscosity solvent blend could enhance slurry stability and, in turn, improve electrode uniformity during fabrication. • The mixture did not obtain the expected result; it caused a phase separation between powders and the rest of the slurry to happen. While the slurry itself was in fact more viscous the phase separation rendered this useless. The test was repeated two times to confirm this strange behaviour.	

After these first, fruitless attempts, a new recipe was tried that was not directly obtained from literature for MCFC electrodes, but generic for nickel-based tape casting slips, and this had a completely different starting recipe then the one tried before, and can be seen in Table 4-7.

Table 4-7 Recipe based on different casting processes, non specific for MCFC electrode casting [96].

<i>Role in the mixture</i>	Compound	Weight distribution:
<i>Base powder</i>	Ni	80 %
<i>Solvent 1</i>	Xylene	7 %
<i>Solvent 2</i>	Ethanol 95%	7 %
<i>Dispersant</i>	Fish Oil	2 %
<i>Binder</i>	Butvar B-98	2 %
<i>Plasticizer</i>	Butylbenzyl Phtalate	2%

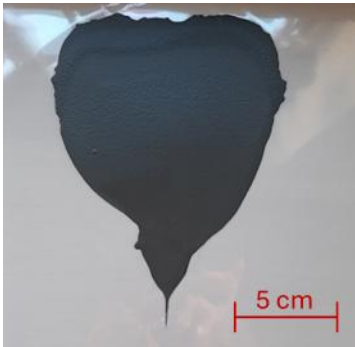
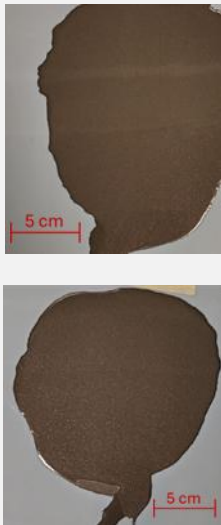
This recipe has a significant higher number of powders compared to the previous recipes and switches the PEG for Butylbenzyl Phtalate. Although the phthalate-based plasticiser raises safety concerns, it was retained initially to establish a clear benchmark; alternative compounds were considered only after a reference formulation had been defined. Another difference when comparing the recipe to the previous ones is the reduced times, which are 5h + 24h, where the first phase is used to dissolve the plasticizer in the solvents and the powders are added in a second phase.



Figure 4-20 Electrode 4, produced through the new recipe. A slight phase separation can be seen in the bottom, but the middle part of the tape was looking good, smooth and without wrinkles.

The result in Figure 4-20 shows a highly dense, dark tape; it was powdery to the touch and excessively thick. This suggests that the solvent, binder, and plasticizer contents were insufficient to effectively bind the overall solid loading in the slurry. Nevertheless, the outcome was encouraging, as the formulation provided a viscosity within a suitable range for efficient tape casting. Accordingly, a subsequent experimental campaign was conducted using this formulation as the starting point, and the results are summarized in Table 4-8.

Table 4-8 Reassuring table of the main results obtained by the production of electrodes 7 to 35

Number	Differences and considerations	Image
7	• The main issue with second recipe was the amount of powder therefore testing was done to evaluate the correct amount of powder • A significant decrease of the powder showed a very promising green sheet production, that was ready to be evaluated with sintering and analytical techniques later	
8 - 35	• After sintering and analysis, utilising SEM imaging and porosimeter the result for electrode 7 showed important potential, so therefore, different experiments were done. These included the variation of the solvents, the binder, the mixing times, and the inclusion of additives. • It was possible to decrease the production time (going from 24h + 24h to 5h + 24h) and change the solvent, but it was not possible to modify the binder plasticizer couple yet, even though as discussed, the phthalate is an issue.	

As mentioned before, the main requirement after production and evaluation of the electrodes was the sintering process. Without sintering the green tape was not indicative of the final product.

The sintering process was studied subsequently to the production of the electrode 7 and starting from literature [87] a homemade process was developed that included three steps. Firstly, the electrode was deposited on a ceramic inert organic compound as a support. The support does not react with the electrode but allows to avoid the electrode sticking to the furnace itself. Then the three heating steps start that are: a first heating up to 200°C, to release the organics in air, then the gases are switched to nitrogen and hydrogen and heated up to 400°C, in the end a last heating up to 800°C is done to complete the sintering process. While it is theoretically possible to remove the whole organic species from the electrode with a reducing temperature using longer explosion times, using oxygen in the first oxidation step has the advantages of being less expensive and guaranteeing the removal of all carbon deposits. The times of the dwelling and even the gases were subject to extensive studies.

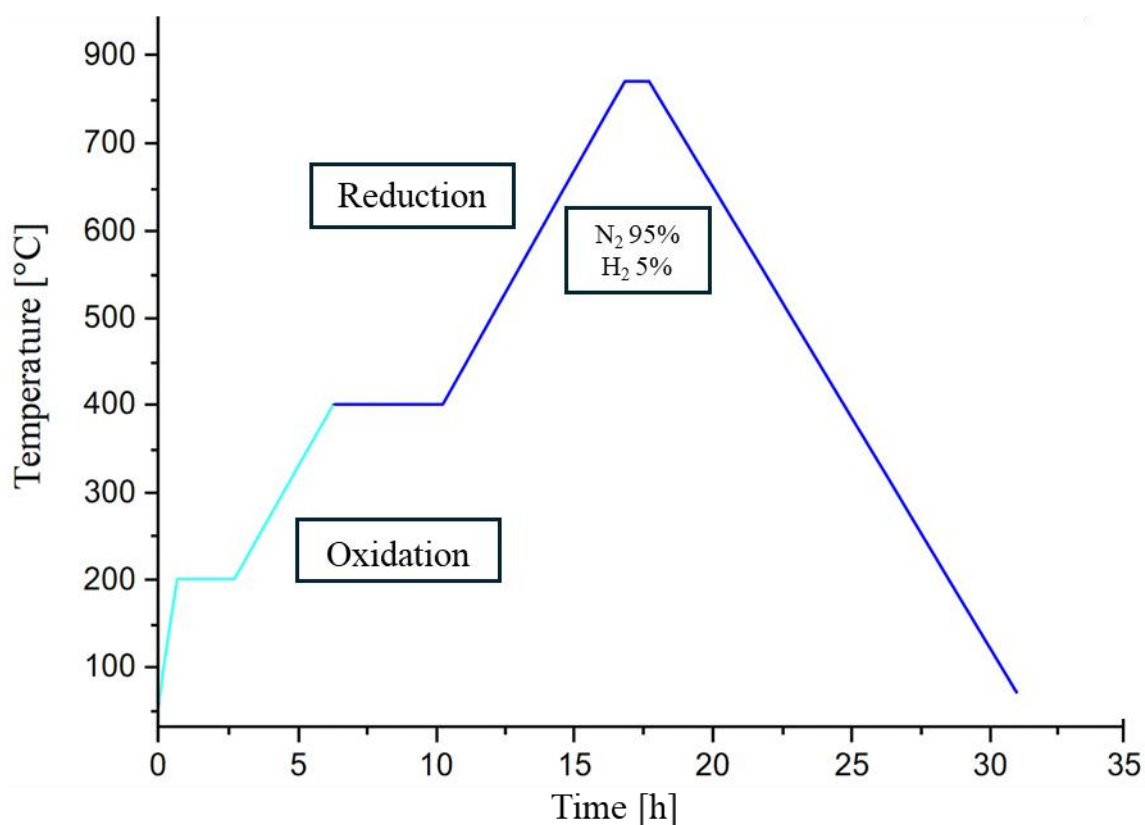


Figure 4-21 Sintering diagram for electrodes, the temperature steps are fixed, as they are required for the controlled burn out of the organics, while the time steps are still subject to extensive studies

After the sintering steps seen in Figure 4-21 the green tape was transformed into a solid metallic slab, and the colour of the slab suggested no oxidation had occurred, as the oxide of nickel, being either NiO or Ni₂O₃, both present distinguishable colouring to the not oxidized metallic nickel.

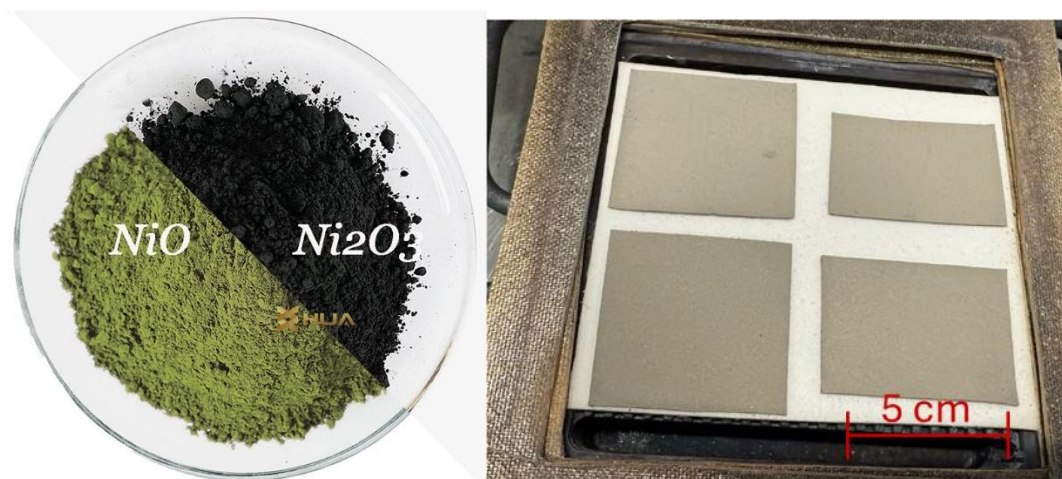


Figure 4-22 On the left the typical colours of the two species can be seen, NiO is distinctly green and Ni_2O_3 is greyish, black [119], on the right the results of the sintering process, visibly distinguished from the Ni – oxide.

As seen in Figure 4-22, the metallic slabs have a distinctly light grey coloration and presented a significant anelastic behaviour, as expected. Having obtained the good samples, these were analysed using SEM imaging.

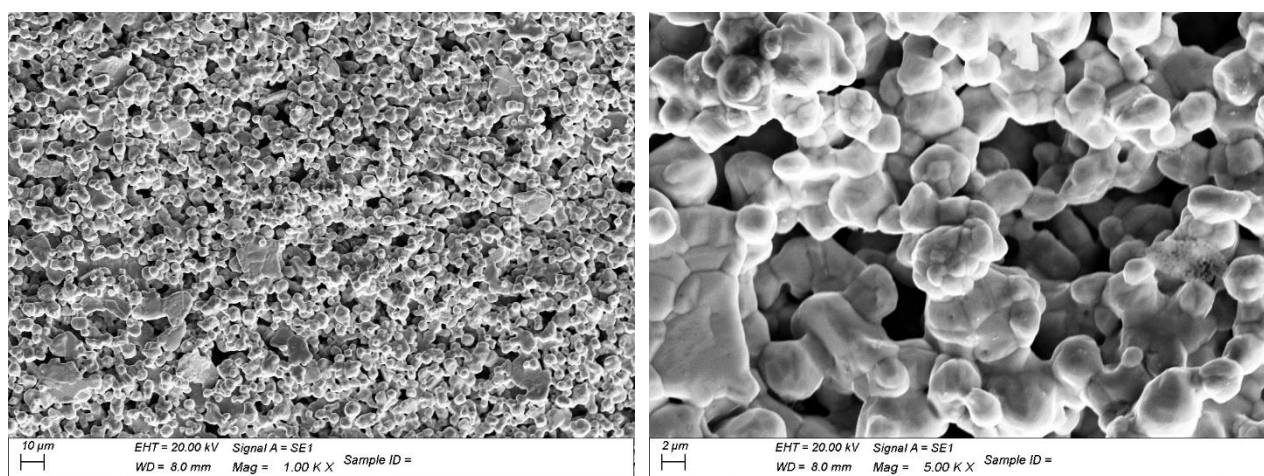


Figure 4-23 SEM analysis of electrode 7 with magnifications 1000 x on the left and 5000 x on the right.

SEM imaging in Figure 4-23 showed a good pore size for the analysed sample around 3 micron and a good apparent porosity of around 3 microns, which suggested a good degree of sintering. This microstructural assessment suggested that the produced electrode was more suitable for anode operation. In the cathodic environment, nickel-containing structures are prone to oxidation and coarsening effects that can progressively reduce open porosity; therefore, starting from an already fine pore network would increase the risk of pore closure and transport limitations during operation. For this reason, the material was first tested as an anode, where the reducing atmosphere is more compatible with maintaining the porous structure. At this stage, no additional catalytic or structural additives were introduced due to toxicity and cost considerations. Since the electrode is primarily nickel-based and nickel provides the main catalytic functionality in MCFC electrodes, the base material can in principle be employed on either side; however, the initial validation was deliberately performed on the anode side to minimise oxidation-driven microstructural degradation and to obtain a more reliable performance assessment.

The next points that will be tackled are on the side of the production the removal of the phthalate, while on the side of the sintering the thing that still must be studied is the time to optimise the pore size, as the process and the degree of sintering are the major drivers for the pore size distribution. Doing this, it could be possible to reach the desired microstructure to use the electrodes also as effective cathodes

4.2.3 Summary of main component results

Both for the matrix as for the electrodes some preliminary components have been obtained, some have also been tested and will be discussed in the next chapter, in Table 4-9 the main characteristics from literature have been compared to the obtained results from the experimental campaigns, considering only the best results:

Table 4-9 Reassuring table of the main results obtained by the production of components at Caplab compared to literature values [72], [73][74][82][84]

Characteristic	Literature - Matrix	Caplab - Matrix	Literature – Anode	Caplab - Anode
<i>Porosity</i>	30 – 70 %	55 - 70 %	55 %	30 - 60 %
<i>Pore size</i>	>1 μm	0.01 – 0.5 μm	3 – 6 μm	1 - 5 μm

4.3 Cell testing

While material synthesis and characterisation are fundamental to the development of MCFCs, they must be complemented by rigorous electrochemical testing, which serves as the definitive assessment of component performance within operational conditions. Cell testing not only validates the functional viability of the materials but also provides critical insights into their behaviour under the dynamic environment of an operating fuel cell.

In Caplab, two kinds of cell dimensions can be tested as seen in Figure 4-25, being 10 cm x 10 cm and 3 cm x 3 cm. The bigger scale is closer to the real-life application, and therefore more useful to analyse the scale up potential of the MCFC. At the same time, a 10 cm x 10 cm test requires more material than smaller scale testing and longer start up times. It must be remembered that the matrix is put inside the cell as a green tape and must sinter in cell Figure 4-24, this sintering requires more time, the bigger the matrix itself is.

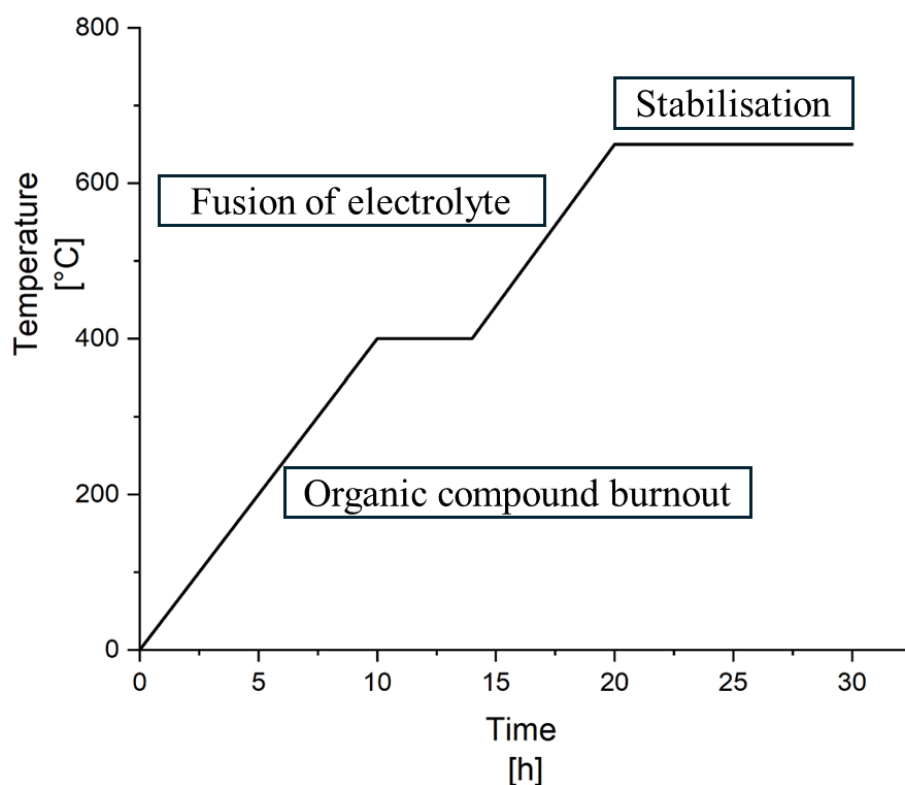


Figure 4-24 Generic start-up procedure for MCFC, the first plateau is dedicated to the oxidation of the organic compounds present inside the matrix

Therefore, the smaller frame, as it allows for faster cell startup and at the same time also to use less material, making it better for material screening. A potential limitation of the small frame is that, as the active cell area decreases, edge regions account for a larger fraction of the total surface, thereby increasing the influence of edge effects. This effect does not translate directly to the scale up and has therefore to be considered when doing small cell testing.



Figure 4-25 On the left two cell frames 10 cm x 10 cm, on the right two cell frames with the cell already positioned and 3 cm x 3 cm dimensions.



Figure 4-26 Cell setup in a 10 cm x 10 cm setup, from left to right we have a current collector (a), then the anode (b), then multiple layers of matrix and electrolyte powders (c + d), and in the end the cathode (e). Usually, the anodic side electrode is put on the bottom, and the cathode is on top.

The preferred order in the case of Caplab testing for a cell frame set-up is as follows, going from the bottom to the top, as seen in Figure 4-26 and Figure 4-27:

- Current collector
- Anode
- Matrix: Depending on the testing setup, one or more sheets can be used to avoid crossover caused by small imperfection in a single layer.
- Electrolyte: Can be in powder or sheet form, the quantity depends on the porosity of the matrix and the electrodes.
- Cathode
- Current collector

The current collector, which has not been studied in this thesis, has the function of distributing the gases while also favouring contact between the electrode and the cell frame. It is usually made of AISI 316 stainless steel and can come in various geometrical forms, from the simplest, like a grid, to more complex with gas channels [120].

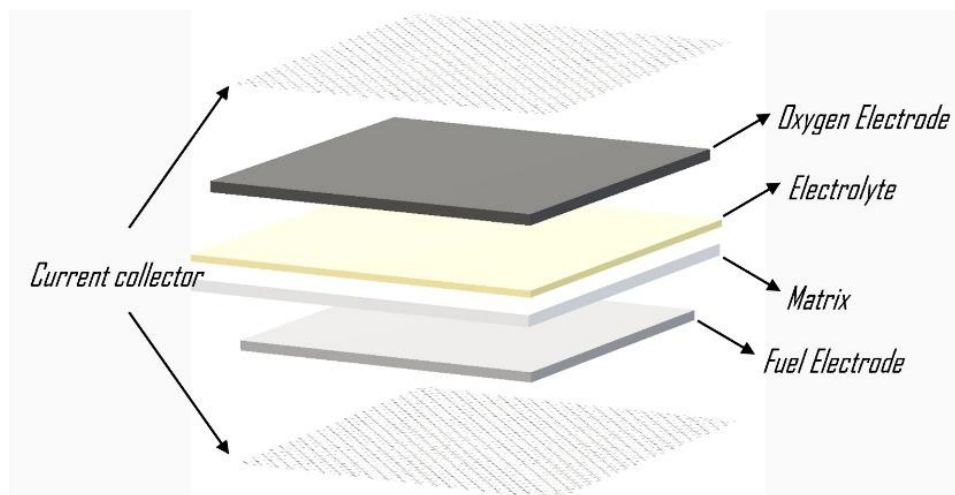


Figure 4-27 Stylised representation of the cell setup.

A critical operation during cell testing is the start – up as many things happen over a short period of time and need to be timed correctly as seen in Figure 4-24. The main stages of the cell testing process are:

- Organic compound burnout:

Depending on binder used and cell dimension this phase can have a differing time and temperature requirements, usually a TGA is performed on the matrix to evaluate the best temperatures to reach. In this phase an air or oxygen flux is required to allow for the combustion to happen.

- Fusion of electrolyte:

The electrolyte fuses at around 500°C depending on the chosen composition [121]. During the fusion, the matrix must be able to favour the intrusion of the liquid electrolyte inside its pores, for it to not flow away, it is therefore of upmost importance that the matrix be completely free of organic compounds by the time the fusion process starts. This phase is particularly critical as the matrix without electrolyte is very brittle. In this phase CO₂ is usually fed on both sides of the cell to avoid electrolyte evaporation. The capillarity of the matrix is very important as it avoids the electrolyte flowing through the electrode and emptying the cell.

- Cell stabilisation and improvement:

This happens when the cell is already fed with its final gas compositions and is already operational. The final gas compositions is on the cathodic side dirty air, meaning a composition of CO₂ at varying percentages (4% up to 30% [122], [123], [124]) with the rest being O₂ and N₂. For the anodic gas composition there are three components: H₂, CO₂, H₂O. These compounds are all necessary, hydrogen is the cell fuel and usually the most present compound inside the fuel gas at around 60-70% for optimal performance, yet can go down to 20% [125], [126]. The presence of CO₂ is important as it inhibits the evaporation of the carbonate by increasing the presence of CO₂ molecules particularly in the inlet, the steam on

the other hand is very important as the cell conditions could favour the deposit of carbon inside the tubes or cell itself through the Boudouard reaction [127]:



The monoxide is produced through the reverse water gas shift reaction, using steam it is possible to avoid the formation of the monoxide whilst also producing more hydrogen [128]:



Both H₂O and CO₂ have a usual percentage of around 10 – 15%, and it is not recommended to go below for the afore mentioned reasons [129].

At Caplab a total of 18 single cells and 12 small frame cells have been tested. Each test had its different choice of materials and was used to determine something else regarding the setup or material performance. The main aims were twofold: checking the performance of homemade materials and checking the possibly to repurpose industrial materials for MCFC application. In the following tables the main results of each test are discussed. It must be noted that the setup of the laboratory still presents some issues that could be related with the relatively short lifespan of the practical lab experience, given by its recent set-up. Introducing the cell testing it is necessary to remember which are the performance targets of the MCFC:

- Power density [130]: 120 mW/cm²
- Open Circuit Voltage [131]: 1.23 V @650°C with a gas composition of 0.84:0.16 H₂:N₂ at the anodic compartment and at the cathode 0.33:0.67 O₂:CO₂

It has also to be stated that particularly the OCV can also differ depending on many factors as temperature, gas composition and cell design, without necessarily compromising the overall cell performance [78].

The main results obtained during testing at Caplab have been resumed into Table 4-10 for full scale cell testing and Table 4-11 for small frame cell testing.

Table 4-10 Single cell testing history with materials used and main results

Cell name	Materials used		Main results
1. Cell_WTU_001	Anode	Commercial product from WTU	- First cell done with materials from academic partners. - The cell suffered a flooding caused by incorrect connection of tubing for the gas humidifiers.
	Cathode	Commercial product from WTU	
	Matrix	Commercial product from WTU	
	Electrolyte	Commercial product from WTU	
2. Cell_Caplab_001	Anode	Commercial product from WTU (reused from test 1 after drying)	- Same electrodes as test one, but different matrix and electrolyte. - No OCV was measured, which was expected as the materials were far from optimal, but it was possible to evaluate at least a correct functioning of the gas lines.
	Cathode	Commercial product from WTU (reused from test 1 after drying)	
	Matrix	Caplab matrix	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
3. Cell_Capab_002	Anode	Commercial nickel mesh from an Italian producer	- First test with alternative materials. - Potential was measured at 0.68 V (target 1.23 V), with a fast decrease.
	Cathode	Commercial nickel mesh from an Italian producer	
	Matrix	Caplab matrix	

Cell name	Materials used		Main results
	Electrolyte	Powder Li K (62 – 38%) carbonate	This behaviour is because of insufficient pressure on the cell and therefore an insufficient contact of the components [132].
4. Cell_WTU_002	Anode	Commercial product from WTU	Potential was obtained again at 0.65 V, suggesting a similar issue to the test before.
	Cathode	Commercial product from WTU	This test was the first one the GC was tried on, using the sampling pump of the instrument a depression was caused that ruptured the matrix, causing the test to stop.
	Matrix	Commercial product from WTU	
	Electrolyte	Commercial product from WTU	
5. Cell_Caplab_003	Anode	Commercial nickel mesh from a Chinese producer	In this test all components were substituted with commercial counterparts.
	Cathode	Commercial nickel mesh from a Chinese producer	The OCV was recorded at 0.48 V, suggesting a non-operational behaviour of the cell.
	Matrix	Commercial matrix	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
6. Cell_WTU_003	Anode	Commercial product from WTU	No potential was measured beside background noise ($\sim \pm 10$ mV).

Cell name	Materials used		Main results
	Cathode	Commercial product from WTU	Even in post-test analysis no visible issue was discovered, and no cross over of the gases was visible. It suggested an issue in the components themselves.
	Matrix	Commercial product from WTU	
	Electrolyte	Commercial product from WTU	
7. Cell_Caplab_004	Anode	Commercial nickel mesh from an Italian producer	- In this test all components were substituted with commercial counterparts, same as 003. - The OCV was recorded at 0.73 V, suggesting a non-operational behaviour of the cell.
	Cathode	Commercial nickel mesh from an Italian producer	
	Matrix	Commercial matrix	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
8. Cell_KIST_001	Anode	Commercial product from KIST	- In this test all components were from KIST. - The OCV was recorded at 0.92 V, suggesting just a slight contact issue, over time this issue increased, probably because of corrosion and caused a short circuit.
	Cathode	Commercial product from KIST	
	Matrix	Commercial product from KIST	
	Electrolyte	Commercial product from KIST	

Cell name	Materials used	Main results
9. Cell_Caplab_005	Anode	Commercial nickel mesh from a Chinese producer
	Cathode	Commercial nickel mesh from a Chinese producer
	Matrix	Commercial matrix
	Electrolyte	Powder Li K (62 – 38%) carbonate
10. Cell_KIST_002	Anode	Commercial product from KIST
	Cathode	Commercial product from KIST
	Matrix	Commercial product from KIST
	Electrolyte	Commercial product from KIST
11. Cell_Caplab_006	Anode	Commercial nickel mesh from a Chinese producer
	Cathode	Commercial nickel mesh from a Chinese producer
	Matrix	Caplab matrix (3 sheets)

Cell name	Materials used	Main results
12. Cell_Caplab_007	Electrolyte	Powder Li K (62 – 38%) carbonate
	Anode	Commercial nickel mesh from a Chinese producer
	Cathode	Commercial nickel mesh from a Chinese producer
	Matrix	Caplab matrix (4 sheets)
13. Cell_Caplab_008	Electrolyte	Powder Li K (62 – 38%) carbonate
	Anode	Commercial nickel mesh from a Chinese producer
	Cathode	Commercial nickel mesh from a Chinese producer
	Matrix	Caplab matrix (3 sheets)
	Electrolyte	Powder Li K (62 – 38%) carbonate
	Anode	Commercial nickel mesh from a Chinese producer
	Cathode	Commercial nickel mesh from a Chinese producer
	Matrix	Caplab matrix (3 sheets)

Cell name	Materials used		Main results
14. Cell_Caplab_009	Anode	Commercial nickel mesh from a Belgian producer	- The OCV was recorded at 1.05 V. - The pattern of slowly decreasing performance was still present. - A power density peak of 10 mW/cm² was reached. - The instability still suggests the need for increased pressure and optimisation of cell contact.
	Cathode	Commercial nickel mesh from a Belgian producer	
	Matrix	Caplab matrix (2 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
15. Cell_Caplab_010 (replicability of the test before)	Anode	Commercial nickel mesh from a Belgian producer	- The OCV was recorded at 1.08 V. - The pattern of slowly decreasing performance was still present. - A power density peak of 5 mW/cm² was reached.
	Cathode	Commercial nickel mesh from a Belgian producer	
	Matrix	Caplab matrix (2 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
16. Cell_Caplab_011 (replicability of the test before)	Anode	Commercial nickel mesh from an Italian producer	- Increased sealing pressure. - Test used for GC calibration; no performance was obtained.
	Cathode	Commercial nickel mesh from an Italian producer	
	Matrix	Caplab matrix (2 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	

Cell name	Materials used		Main results
17. Cell_Caplab_012	Anode	Commercial nickel mesh from a Chinese producer	- Increased sealing pressure, 0.6V. - Stable performance. - The electrodes did probably not have the correct pore size for the required task.
	Cathode	Commercial nickel mesh from a Chinese producer	
	Matrix	Caplab matrix (2 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
18. Cell_Caplab_013	Anode	Commercial nickel mesh from a Chinese producer	- Increased sealing pressure, 0.5V. - Stable performance. - No electrolyte retention, pores too big and no capillarity was achieved.
	Cathode	Commercial nickel mesh from a Chinese producer	
	Matrix	Caplab matrix (2 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	

Table 4-11 Small frame cell test with materials used and main results

Cell name	Materials used		Main results
1. Cell_Small_001	Anode	Commercial nickel mesh from an Italian producer	- The first small cell was done with commercial materials, both to test the set-up having seen the results of the first big cell test and not waste good material from other companies. - Stable cell performance at 0.9 V, drop-off caused by broken humidifiers.
	Cathode	Commercial nickel mesh from an Italian producer	
	Matrix	Caplab matrix (4 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
2. Cell_Small_002	Anode	Commercial product from WTU	- Replicability done with materials from WTU. - No performance was reached, 0.65 V of OCV but immediately decreased drastically over a short time frame.
	Cathode	Commercial product from WTU	
	Matrix	Commercial product from WTU	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
3. Cell_Small_003	Anode	Commercial product from WTU	- Same electrodes as before but different matrix to see if that was the issue. - Same performance reached with fast decrease, 0.65 V peak.
	Cathode	Commercial product from WTU	
	Matrix	Caplab matrix (4 sheets)	

Cell name	Materials used	Main results
4. Cell_Small_004	Electrolyte	Powder Li K (62 – 38%) carbonate
	Anode	Commercial product from WTU
	Cathode	Commercial product from WTU
	Matrix	Caplab matrix (2 sheets)
5. Cell_Small_005	Electrolyte	Powder Li K (62 – 38%) carbonate
	Anode	Commercial product from WTU
	Cathode	Commercial product from WTU
	Matrix	Caplab matrix (2 sheets)
6. Cell_Small_006	Electrolyte	Powder Li K (62 – 38%) carbonate
	Anode	Commercial product from WTU
	Cathode	Commercial product from WTU
6. Cell_Small_006	Matrix	Caplab matrix (2 sheets)

Cell name	Materials used		Main results
7. Cell_Small_007	Electrolyte	Powder Li K (62 – 38%) carbonate	Higher performance peak at 0.8 V, then rupture of the matrix and fall to 0.7 mV, with a progressive decrease.
	Anode	Commercial product from KIST	New kind of electrodes, as the previous were never functional.
	Cathode	Commercial product from KIST	
	Matrix	Caplab matrix (2 sheets)	
8. Cell_Small_008	Electrolyte	Powder Li K (62 – 38%) carbonate	- The cell was stable at 700 mV. - Over time a black deposit was formed, that was identified as carbon, that was deposited because the tube that fed the humidifiers was not completely immersed in the water supply and therefore the gases were dry, favouring the Boudouard reaction [127].
	Anode	Commercial product from KIST	
	Cathode	Commercial product from KIST	
	Matrix	Caplab matrix (2 sheets)	
9. Cell_Small_009	Electrolyte	Powder Li K (62 – 38%) carbonate	Voltage increased and kept steady at 700 mV.
	Anode	Commercial product from WTU	

Cell name	Materials used		Main results
	Cathode	Commercial product from WTU	During operation, moving the setup produced an increase to 750 mV suggesting an instable cell setup.
	Matrix	Caplab matrix (3 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
10. Cell_Small_10	Anode	Commercial product from WTU	- Replicability of the before see if a more meticulous cell preparation process could increase the cell potential. - The result was worse than the previous test, reaching 550 mV, that can be cause by the rupture of the matrix.
	Cathode	Commercial product from WTU	
	Matrix	Caplab matrix (3 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
11. Cell_Small_11	Anode	Caplab anode	- Cell increased up to 0.92V. - Stable at around 0.9V, with a discrete power output around 20 mW/cm². - An alignment issue of the two halves of the cell frames was to blame, moving the frames the performance improved.
	Cathode	Commercial product from WTU	
	Matrix	Caplab matrix (3 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
12. Cell_Small_12	Anode	Commercial nickel mesh from a Chinese producer	The commercial material was much softer than a normal anode.

Cell name	Materials used		Main results
13. Cell_Small_13	Cathode	Commercial product from WTU	During operation, through compression, the cell lost contact and only reached a peak performance of 0.42 V.
	Matrix	Caplab matrix (3 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	
	Anode	Commercial product from WTU	- A new kind of insulation material was used; this could potentially allow to increase the contact stability. - The cell reached a peak of 1 V and was able to provide around 20 mW of power, which is more than usual, but a fast decrease in cell performance caused the shutdown of the system.
	Cathode	Commercial product from WTU	
	Matrix	Caplab matrix (2 sheets)	
	Electrolyte	Powder Li K (62 – 38%) carbonate	

4.3.1 Research secondment at KTH

A research secondment was carried out at the KTH Royal Institute of Technology (Stockholm), where MCFC single cell testing procedures and facilities are well established. This activity was used to benchmark the materials developed in this work under a mature and reproducible test rig, thereby complementing the ongoing testing campaign at the University of Genoa and strengthening the overall validation.

A total of six different cell tests were done, with significant results. There were some differences between the setup at Caplab and the one at KTH, the cell dimension was smaller, being a round 3 cm² cell, called commonly a button cell. Furthermore, the furnace was open and not closed like the setup in Genova, with a simplified access to the hearth of the cell. The cell is located inside two concentric ceramic tubing, where the internal tube is responsible for the gas flow towards the cell and the external one for the exit. The current collector is directly connected with the outside using a long metal rod welded on to it. The tubes are symmetrical, one closing from above, one from below with the cell in the centre. The described set up has been schematically shown in Figure 4-28.

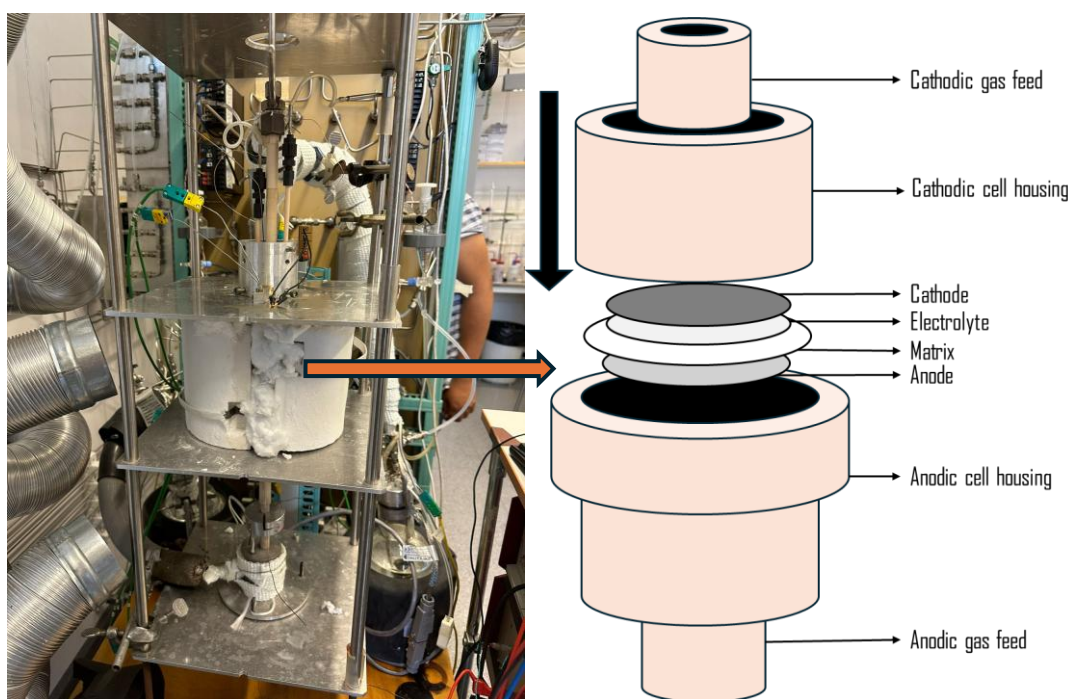


Figure 4-28 Bottom cell setup at KTH, on the left a picture of the closed setup, on the right the configuration of the button cell inside the ceramic frame that is heated inside the muffle furnace.

The six test were dedicated to testing matrix performance, as it was the component that had been studied the most up to this point. In particular, the first test was done as mentioned during the matrix chapter with the recipe Caplab 1, which showed the best compatibility with the literature KPIs with the porosity around 60% and pore size of 0.16 micron. The remainder of the components used inside the cell setup were proven benchmark components from KTH.

The first test showed high performance, reaching the target of 120 mW/cm². This already gave indications to the fact that the set-up in Genoa was not working correctly as even the commercial electrodes were not

operating. The test conditions were gas compositions of 16/64/20 CO₂/H₂/H₂O at the anode side and 30/15/55 CO₂/O₂/N₂ saturated in a humidifier at 30°C at the cathode side. The startup procedure that was done, and repeated for all subsequent test, was 8h long, with one intermediate step at 450°C to allow for complete organic release. A 2 kg weight was placed on top of the cathodic side electrode.

Cell performance was assessed once 650°C was reached by combining polarisation (I–V) curves and electrochemical impedance spectroscopy (EIS). The I–V curve provides a direct measure of voltage response under load and is expressed with the power density curve as described in Equation 1.

$$P \left[\frac{mW}{cm^2} \right] = V [V] \cdot j \left[\frac{mA}{cm^2} \right] \quad \text{Equation 1}$$

It allows comparison of operating range and peak performance. In parallel, EIS was used to support interpretation of the observed losses by separating resistive contributions that cannot be uniquely distinguished from I–V curves alone. EIS results are reported as Nyquist plots, where the real component Z' is plotted on the x-axis and the imaginary component $-Z''$ on the y-axis. In this representation, the high-frequency intercept on the real axis corresponds to the ohmic resistance R_Ω (electrolyte conduction and contact contributions), while the low-frequency intercept corresponds to the total resistance R_{tot} ; the difference between the total resistance and the ohmic resistance is the overall polarisation resistance R_{pol} associated with kinetic and mass-transport effects.

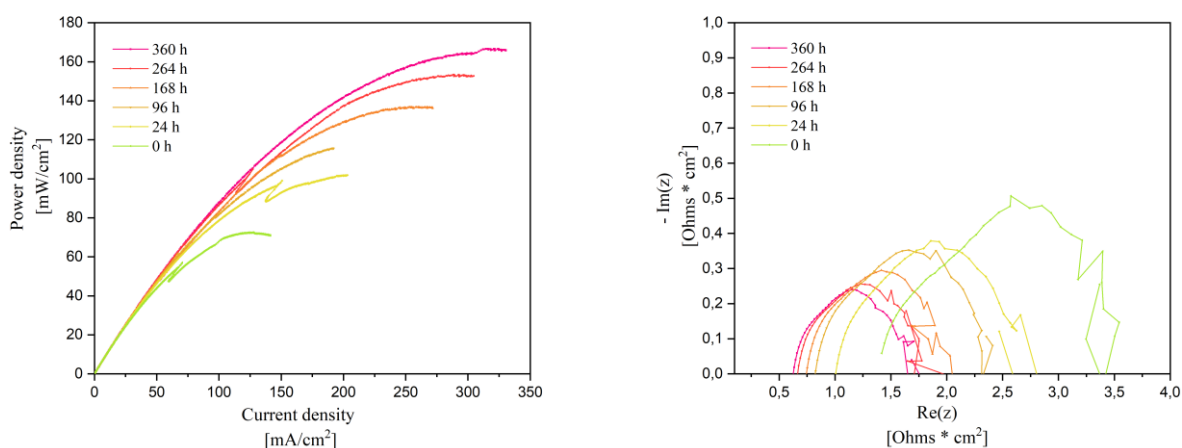


Figure 4-29 Cell test 1 at KTH. Using Caplab 1 and reference conditions. On the left the power density vs current density, on the right the EIS spectra have been determined during the stabilisation process, showing the evolution over time.

Over time the performance of the cell increases, this is caused by a better distribution of the carbonates inside the cell over time, the optimal condition is reached when the electrolytes completely fill all pores of the matrix and therefore form the maximum amount of ionic conduction from the electrodic compartments, this process also includes the electrodes as the electrolyte then forms the three boundary layer and the better the distribution of the electrolyte over the matrix surface, the better this layer will be. The time required relates to the physical time the electrolyte requires to diffuse into all pores and distribute correctly. This can also be seen by looking

at the EIS analysis in Figure 4-29, which shows a decrease of the internal resistance and a reduction of the polarisation resistance over time. As shown, both the ohmic resistance and the polarisation resistance decrease over time. This behaviour is consistent with progressive stabilisation of the cell, as improved contact between components and a more uniform electrolyte distribution enhance ionic conduction pathways and interfacial effectiveness. In addition, as electrolyte wetting becomes more homogeneous, the availability of open porosity at the electrode–matrix interfaces is stabilised, facilitating the transport of reactants to the active reaction zones (three-phase boundary) and reducing concentration-related losses.

The cell reached a peak performance of 170 mW/cm^2 which is higher than the expected and desired target from literature of 120 mW/cm^2 , which is the value that is considered as the minimum operational threshold required for the cell to be functioning properly.

Seen that the cell performance was stable, it was decided to carry out different tests to evaluate the cell performance in differing temperature and gas conditions. Starting with the temperature, a range between 600°C and 700°C was chosen with an interval of 25°C . For each temperature, the cell was allowed to stabilise before the corresponding polarisation curve was measured.

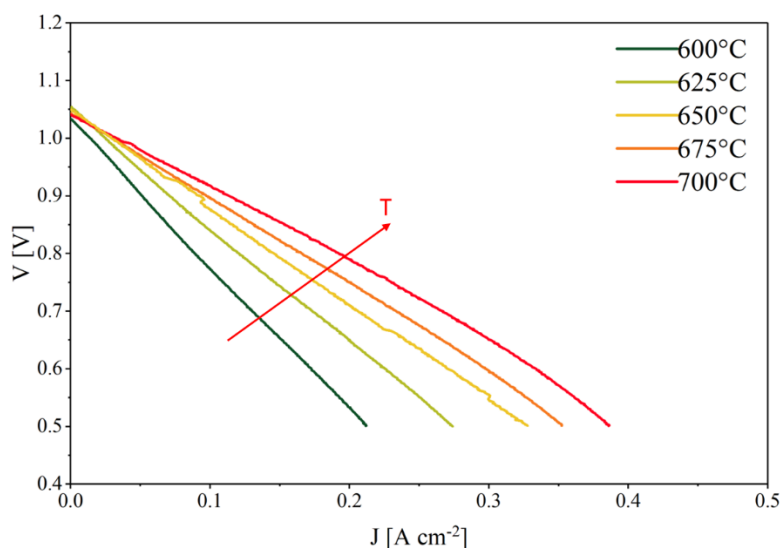


Figure 4-30 Polarization curve Temperature variation

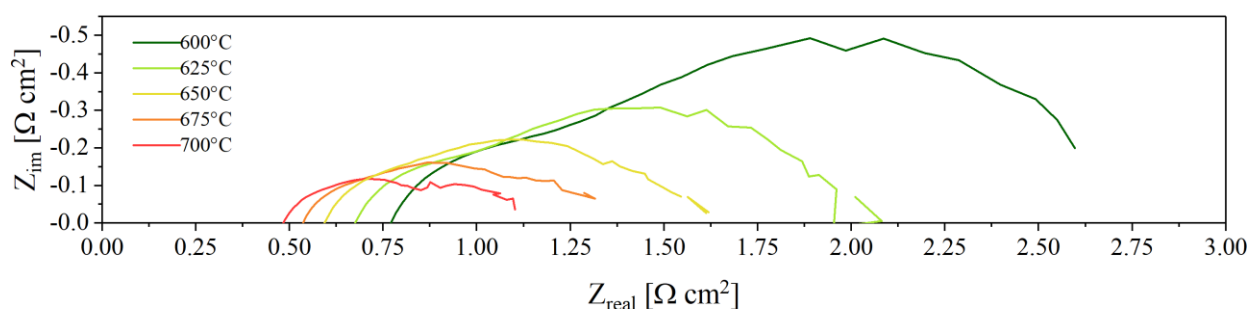


Figure 4-31 EIS curve Temperature variation

As expected, the temperature increase caused also an improvement in internal resistance and cell performance as seen in Figure 4-30 and Figure 4-31. What cannot be seen here is that the degradation process inside the cell at high temperature was significantly higher as the evaporation rate of electrolytes sensibly increased, as discussed previously this being one of the main causes for rapid cell aging. The effect has purposely not been reached as the aim was to avoid having to interrupt the cell test operation.

The second experimental series that was done was on evaluating the effect of gas variation on cell performance. Here the focus was set on the cathodic gas composition and particularly the study of low carbon content and low oxygen content gas compositions as seen in Table 4-12.

Table 4-12 Composition table for cathode and anode gases in the series of gas changes to evaluate the effect of oxygen and CO₂ concentrations.

			Anode	Cathode
			CO ₂ /H ₂ /H ₂ O	CO ₂ /O ₂ /H ₂ O/N ₂
A	CO ₂ , Cathode effect [vol%]	1	16.0/64.0/20.0	5.0/15.0/4.0/76.0
		2		10.0/15.0/4.0/71.0
		3		15.0/15.0/4.0/66.0
		4		20.0/15.0/4.0/61.0
B	CO ₂ , Cathode effect [vol%]	1	16.0/64.0/20.0	5.0/30.0/4.0/61.0
		2		10.0/30.0/4.0/56.0
		3		15.0/30.0/4.0/51.0
		4		20.0/30.0/4.0/46.0

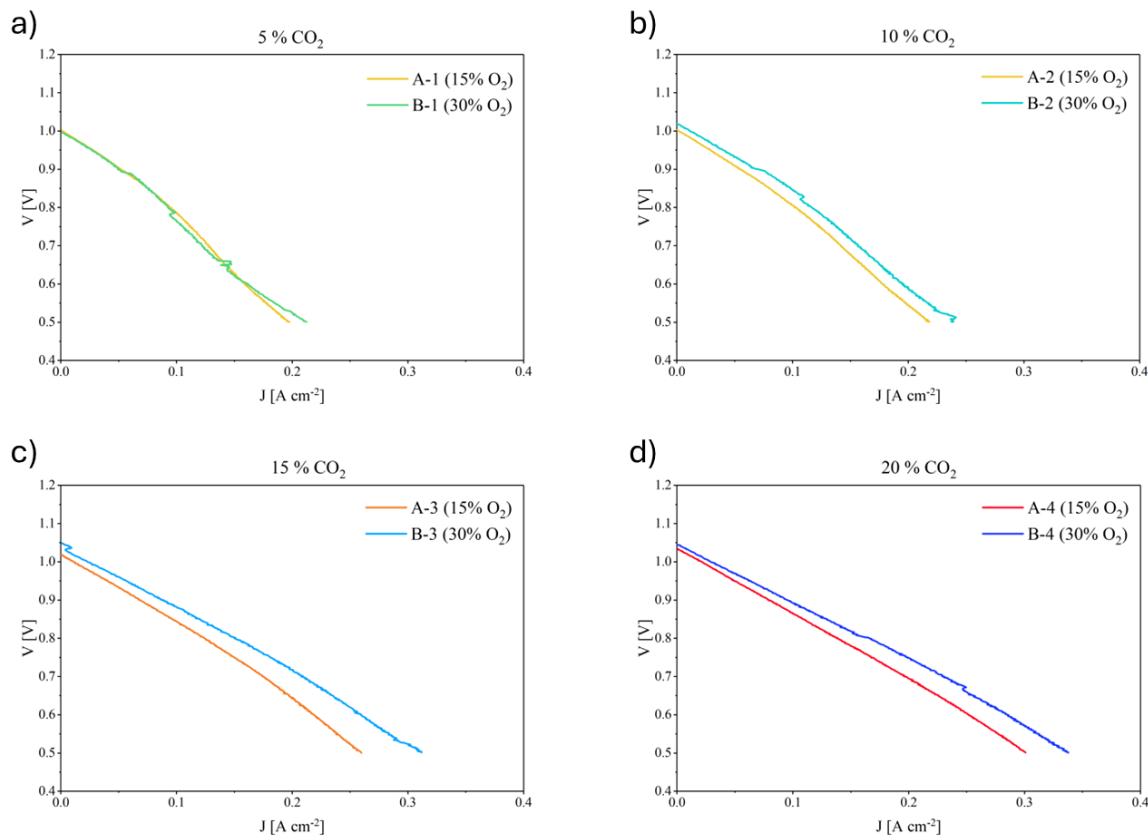
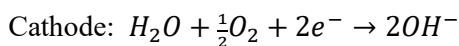
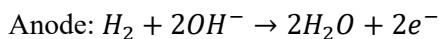


Figure 4-32 Polarization curves obtained by changing CO_2 and O_2 content of the cathodic gases.

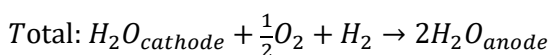
From the changes described in Table 4-12, the low CO_2 effect with less oxygen was much more notable as described in Figure 4-32. Particularly, the 5% CO_2 composition (a) showed that having a higher oxygen content was able to stop the IV curve from dropping towards higher current densities as there is a trend upwards again, this can be observed well by seeing how the yellow curve continues its drop, while the green one slows down in its decrease. Oxygen can also participate by promoting the formation of the ionic charge carrier hydroxide other than carbonate. This behavior has been described as a dual-ion mechanism, in which carbonate and hydroxide ions can both contribute to charging transport under specific operating conditions. At high current densities, the local CO_2 concentration can become depleted, reducing the availability of a carbonate forming species and thus limiting the dominant carbonate-ion conduction pathway. Under these CO_2 lean conditions, water present in the system can increasingly participate in the electrode reactions, enabling pathways that generate hydroxide ions in the presence of oxygen. The resulting hydroxide migrates through the electrolyte, partially compensating for the diminished carbonate-ion flux and helping to sustain overall ionic conductivity despite reduced CO_2 availability [133].



Half-cell reaction 7



Half-cell reaction 8



Complete reaction 9

The subsequent test was performed using the same component set, while replacing the matrix with an alternative sample produced in Genoa using a different solvent system. This change was not motivated by shortcomings of the Caplab 1 matrix, on the contrary, the first test provided encouraging results, but by practical scheduling considerations and the need to maximise the information gained during the limited testing window. In parallel, a new Caplab 1 matrix from a separate production batch was being prepared in Genoa to assess the replicability of the initial outcome. Therefore, while the second test was carried out with the available solvent-variant matrix (with comparable microstructural characteristics), the replicated Caplab 1 matrix was reserved for a dedicated follow-up test aimed at validating batch-to-batch repeatability. This one was the number M97, yet it had significantly lower performance than the previous one. This could be connected to the fact that the solvent used were significantly more reactive and prone to forming intermediates, which could hinder the overall cell performance. Furthermore, the pore form could have also an effect on the lower cell performance.

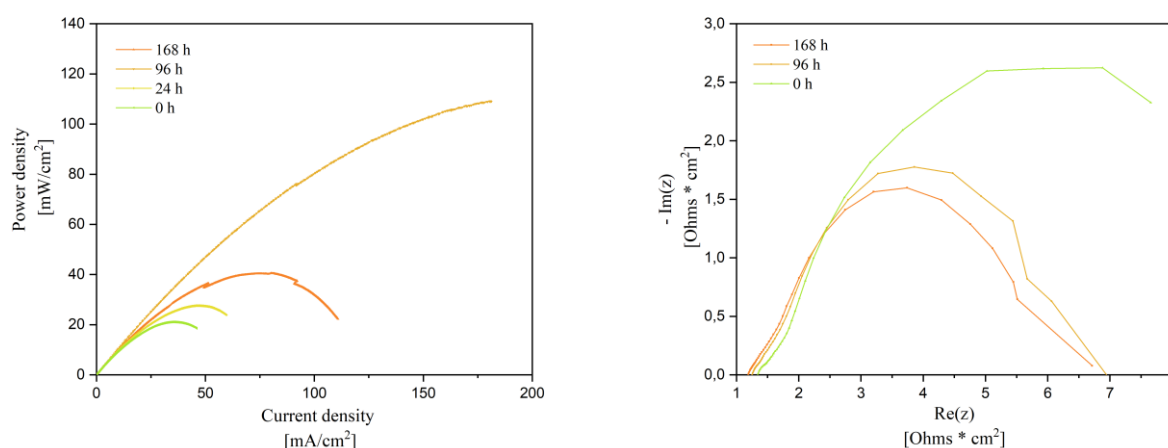


Figure 4-33 Cell test 2 at KTH. Using matrix 97 and reference conditions. On the left the power density vs current density, on the right the EIS spectra have been determined.

The evolution over time of the cell seen in Figure 4-33 shows improvement, but it never reaches the same performance as the cell tested before. Also, the internal resistance decreased but even after the decrease the cell resistance was still very high ($1.26 \Omega \cdot \text{cm}^2$ compared to $0.63 \Omega \cdot \text{cm}^2$ for the previous cell). The shape of the EIS curves also doesn't suggest the same behaviour as the previous cell test as no separate semi circles are visible. It was therefore decided that the cell was to be stopped and a replicability for test one was in order, by producing a new component with the same recipe, but of a different batch, to confirm the good performance obtained from the first sample. As soon as the new matrix was available, the test was initiated. The resulting polarisation and power-density curves were consistent with those obtained in Test 1, confirming the reproducibility of the observed performance within the experimental scatter. In particular, the peak power density was comparable to the reference case, as seen in Figure 4-34.

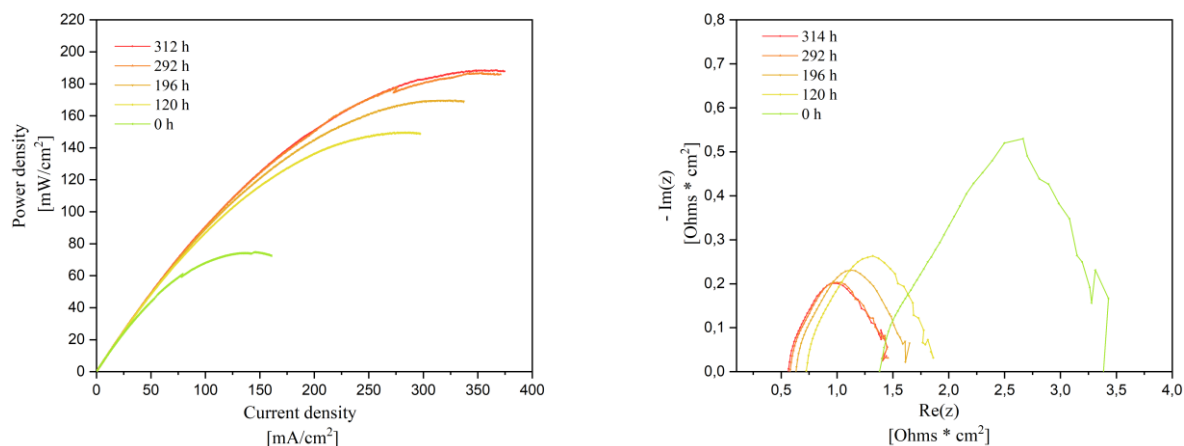


Figure 4-34 Cell test 3 at KTH. Using Caplab 1 and reference conditions. On the left the power density vs current density, on the right the EIS spectra have been determined.

Although the performance in terms of power per square centimetre was higher (up to $200 \text{ mW}/\text{cm}^2$), the internal resistance remained elevated and never reached the target value of $0.63 \Omega \cdot \text{cm}^2$ of the first cell, even if it got close, stopping around $0.66 \Omega \cdot \text{cm}^2$. This was offset by a lower polarization resistance as described by the delta between the intersections of the EIS curve and the $\text{Re}(z)$ axis. This phenomenon has been attributed to a more homogeneous distribution of electrolyte within the cell, which is influenced by the accuracy of the assembly process. A well-controlled assembly promotes uniform electrolyte infiltration and retention across the porous electrode matrix structure, minimizing local depletion or flooding effects. As a result, the reactive zone becomes more evenly utilized and diffusion limitations are mitigated, allowing gaseous reactants to diffuse more effectively throughout the electrochemically active layer and improving access of the reacting species to catalytic sites.

For Cell 4, a different electrode type was tested, namely a commercial felt-like material like that previously evaluated in Genoa. The purpose of this test was to assess whether the poor performance observed in Genoa was primarily attributable to the electrode itself or influenced by test-rig effects as seen with the matrix. By testing the same felt electrode in the established KTH setup, the experiment aimed to provide an external benchmark and to verify whether the material is intrinsically unsuitable for the intended MCFC application.

The results were promising. It reached the operating OCV of 1.06 V, and was also able to provide performance, yet as can be seen in the power density curves in Figure 4-35, it had difficulties towards higher current densities, as if there was a limiting phenomenon that had not been seen in the other cases. The main difference was the dimension of the pores, that was bigger than the ones present at KTH (from SEM imaging at least 10 times bigger). It seemed like the electrode, that was in this case used to substitute the anode, could not retain the three-phase boundary layer correctly. This behaviour is also reflected in the power-density curves: at high current densities the curve develops a slight “hook” given by a decrease in power with increasing load, which is indicative of mass-transport limitation and suggests a reduction in the effective three-phase boundary rather than a purely ohmic effect. Consistently, the EIS results show that the polarisation resistance reaches its minimum at 144 h and then increases at 168 h and 192 h. This trend is most plausibly attributed to electrolyte

depletion or redistribution (leading to reduced ionic connectivity and active area), as the timescale is too short to indicate significant intrinsic material degradation and similar components remained stable over comparable durations in the other tests. What is also interesting is that this cell internal resistance was the lowest tested during the research secondment, yet this advantage was completely lost due to a strong overall polarisation resistance.

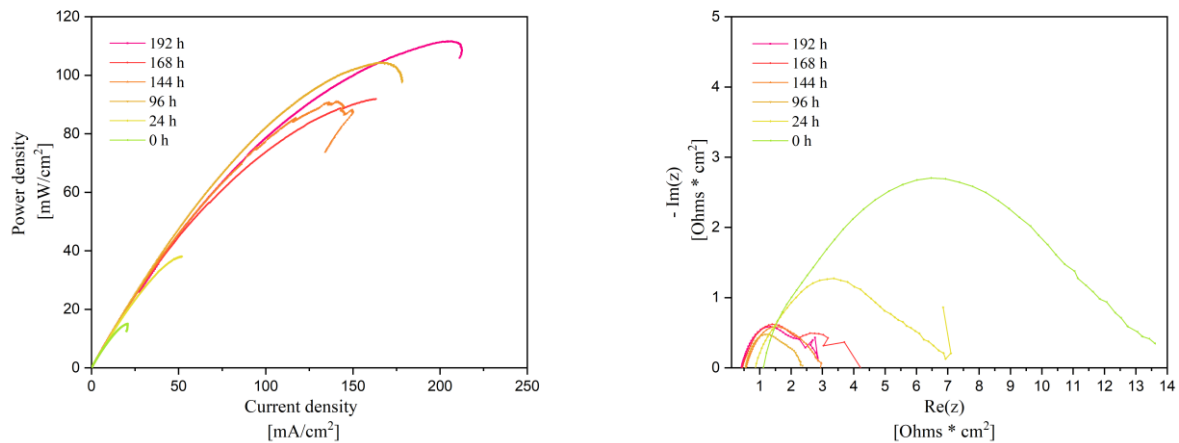


Figure 4-35 Cell test 4 at KTH. Using a different anode and reference conditions. On the left the power density vs current density, on the right the EIS spectra have been determined.

Having seen that the Caplab 1 was able to provide consistent and replicable results, the aim was to see if it was also compatible with different kinds of electrodes. At KTH another couple of anode and cathode from another producer company was available and was tested. Although the detailed composition of these electrodes remains proprietary, the primary disclosed modification concerns their geometry: the thickness of both the anode and the cathode was increased by 0.1 mm relative to the previously used design.

Two tests were made, as during the first test the cell was overloaded at 11 A, causing a drop in the cell performance, probably because of fast carbonate evaporation.

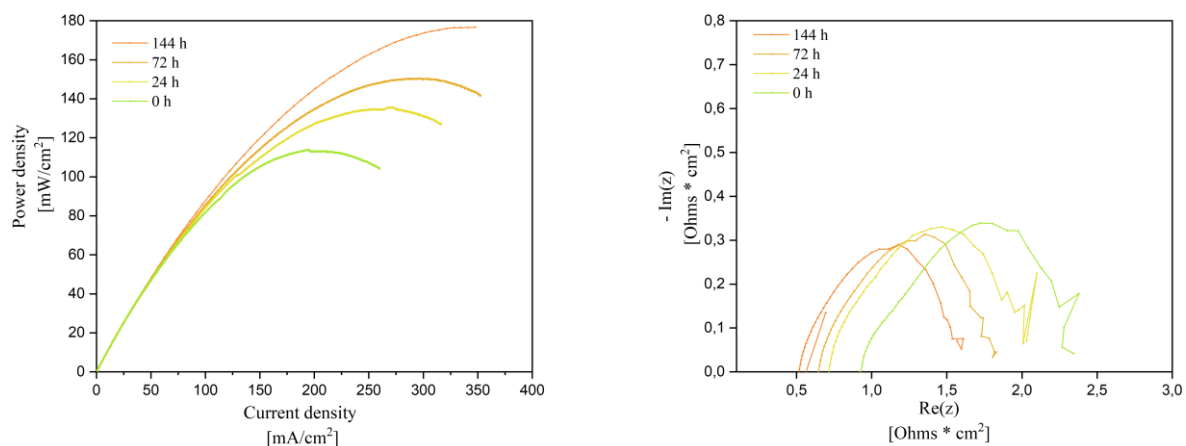


Figure 4-36 Cell test 5 at KTH. Using Caplab 1 and different electrodes at reference conditions. On the left the power density vs current density, on the right the EIS spectra have been determined. Test interrupted due to current overload.

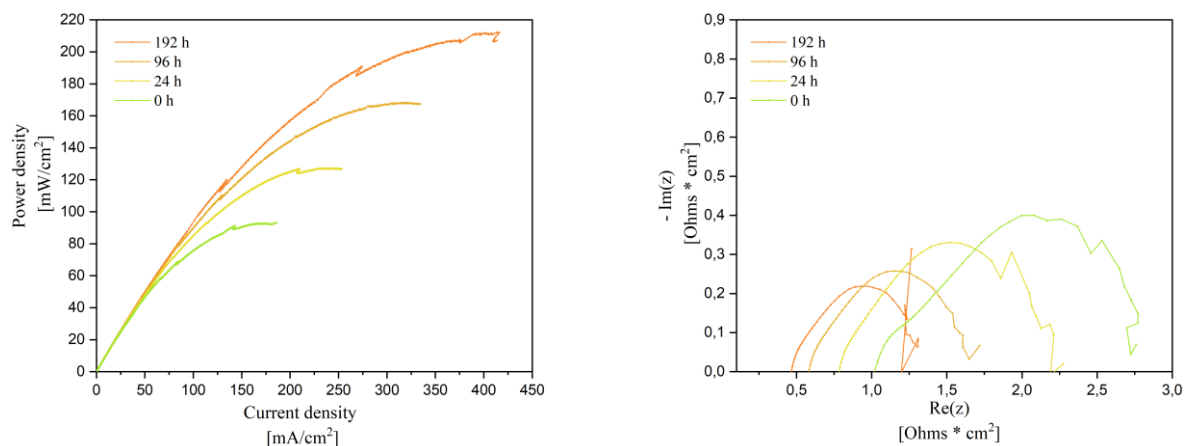


Figure 4-37 Cell test 6 at KTH. Using Caplab 1 and different electrodes at reference conditions. On the left the power density vs current density, on the right the EIS spectra have been determined. Test interrupted due to current overload.

Before the break caused by the current overload, the cell was performing very well, reaching an internal resistance of $0.5 \Omega \cdot \text{cm}^2$ as seen in Figure 4-36, which is lower compared to the ones seen in the first tests with the homemade matrix. A lower resistance also meant a higher power output that reached around $180 \text{ mW}/\text{cm}^2$ before the cell was stopped.

To confirm this performance the same cell test was repeated again, with the results being presented in Figure 4-37, this time leaving the cell more time to diffuse better during the startup, and the results showed that the internal resistance reached as low as 0.46 cm^2 with a peak power output above $210 \text{ mW}/\text{cm}^2$, which is also the best power value obtained using the homebrew matrix.

This experimental campaign produced several relevant outcomes. In particular:

- The comparison between tests performed in Genoa and at KTH indicated that the Genoa testing rig still requires further optimisation, as the same component set led to different electrochemical responses in the two facilities.
- The Caplab 1 matrix, which had previously shown suitable microstructural characteristics, also demonstrated reliable behaviour under real cell operating conditions.
- Matrix M97, despite exhibiting microstructural features comparable to Caplab 1 while being produced with a different solvent system, did not operate satisfactorily in the cell. This result highlights that microstructural analysis can provide useful indications regarding operability, but it cannot, on its own, guarantee electrochemical performance.

Based on these findings, Caplab 1 was adopted as the laboratory benchmark matrix. The subsequent work will therefore focus on producing larger quantities of this formulation to enable extended testing and, in the short term, to support preliminary stack validation (approximately 5–8 cells).

5 Simulation

The first thing that had to be done was to determine the cell parameters that could be used inside the simulation and these have been taken from a previous work of the group [134].

5.1 Electrochemical model

The mechanism that has been proposed considers the equivalent circuit model of the two parallel reactions that are one for the migration of CO_3^{2-} ions (that are responsible for the CO_2 capture) and migration of OH^- ions (that are competitive with the carbon capture). The reactions for both ionic migration paths have been described in Table 5-1.

Table 5-1 Cell reaction for the cathodic, anodic and total cell reaction for both reaction paths of the cell

Carbonate ions migration path	Hydroxide ions migration path
Cathode: $\text{CO}_2 + \frac{1}{2}\text{O}_2 + 2e^- \rightarrow \text{CO}_3^{2-}$	Cathode: $\text{H}_2\text{O} + \frac{1}{2}\text{O}_2 + 2e^- \rightarrow 2\text{OH}^-$
Anode: $\text{H}_2 + \text{CO}_3^{2-} \rightarrow \text{CO}_2 + \text{H}_2\text{O} + 2e^-$	Anode: $\text{H}_2 + 2\text{OH}^- \rightarrow 2\text{H}_2\text{O} + 2e^-$
Total: $\text{CO}_{2,\text{cathode}} + \frac{1}{2}\text{O}_2 + \text{H}_2 \rightarrow \text{CO}_{2,\text{anode}} + \text{H}_2\text{O}$	Total: $\text{H}_2\text{O}_{\text{cathode}} + \frac{1}{2}\text{O}_2 + \text{H}_2 \rightarrow 2\text{H}_2\text{O}_{\text{anode}}$

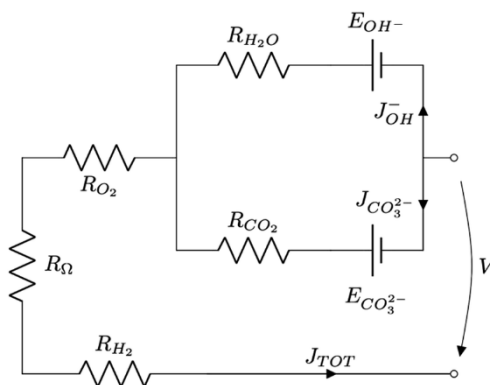


Figure 5-1 Schematic representation of the dual ion mechanism as an equivalent electrical circuit [133], [134]

From the schematic in Figure 5-1, it follows that to describe the MCFC system using the dual-ion model, it is necessary to solve a system that accounts for the fact that carbonate ion transport and hydroxide ion transport are parallel phenomena. This is done by considering the contribution to the overall current as a sum of the contributions of both separate paths.

In particular, the kinetic equation for determining the cell potential V [V] is expressed as:

$$\begin{cases} V = E_{CO_3^-} - J_{CO_3^-} * R_{CO_3^-} - R_{EXT} * J_{TOT} & \text{Equation 2} \\ V = E_{OH^-} - J_{OH^-} * R_{OH^-} - R_{EXT} * J_{TOT} & \text{Equation 3} \\ J_{TOT} = J_{CO_3^-} + J_{OH^-} & \text{Equation 4} \end{cases}$$

E_i – Thermodynamic equilibrium potential, described by the Nernst equation, corresponding to the i -th ion [V]

$R_{CO_3^{2-}}$ – Resistance associated with the cathodic reactant CO_2 [$\Omega \cdot cm^2$]

R_{OH^-} – Resistance associated with the cathodic reactant H_2O [$\Omega \cdot cm^2$]

R_{ext} – Total external resistance of the system, expressed as:

$$R_{ext} = R_{H_2} + R_{O_2} + R_{\Omega} [\Omega \cdot cm^2]$$

R_{H_2} – Resistance associated with the anodic reactant H_2 [$\Omega \cdot cm^2$]

R_{O_2} – Resistance associated with the cathodic reactant O_2 [$\Omega \cdot cm^2$]

R_{Ω} – Ohmic resistance [$\Omega \cdot cm^2$]

J_{tot} – Total current density [A/cm^2]

$J_{CO_3^{2-}}$ – Current density due to carbonate ion transport [A/cm^2]

J_{OH^-} – Current density due to hydroxide ion transport [A/cm^2]

The single contributing variables are calculated locally as follows:

$$E_i = E_0 - \frac{RT}{zF} \prod_i p_i^{v_i} \quad \text{Equation 5}$$

$$R_{CO_2} = -\frac{P_{CO_2,1}T}{J_{CO_3^-}} \ln \left(1 - \frac{J_{CO_3^-}}{P_{CO_2,2} e^{\frac{P_{CO_2,3}}{T}} p y_{CO_2,average}} \right) \quad \text{Equation 6}$$

$$R_{H_2O} = -\frac{P_{H_2O,1}T}{J_{OH^-}} \ln \left(1 - \frac{J_{OH^-}}{P_{H_2O,2} e^{\frac{P_{H_2O,3}}{T}} p y_{H_2O,average}} \right) \quad \text{Equation 7}$$

$$R_{H_2} = -\frac{P_{H_2,1}T}{J_{TOT}} \ln \left(1 - \frac{J_{TOT}}{P_{H_2,2} e^{\frac{P_{H_2,3}}{T}} p \ln(1 + y_{H_2})} \right) \quad \text{Equation 8}$$

$$R_{O_2} = P_{O_2,1} T e^{\frac{P_{O_2,2}}{T}} p^{0.5} \frac{y_{CO_2,average}}{y_{O_2,average}^{0.5}} \quad \text{Equation 9}$$

$$R_{\Omega} = P_{\Omega,1} e^{\frac{P_{\Omega,2}}{T}} \quad \text{Equation 10}$$

E_0 – Standard thermodynamic equilibrium potential [V]

z – Number of electrons involved in the reaction [-]

p_i – Partial pressure of the i -th component [atm]

v_i – Stoichiometric coefficient of the i -th component [-]

F – Faraday constant = 96485 [C/mol]

R – Ideal gas constant = 8.314 [J/(K·mol)]

p – Pressure [atm]

P_i – Fitting parameters related to the i -th component

T – Temperature [K]

y_i – Molar fraction of the i -th component in the bulk

$y_{i, \text{average}}$ – Molar fraction of the i -th component averaged over the bulk–reaction site thickness

The system of equations described involves four variables: V , $J_{\text{CO}_3^{2-}}$, J_{OH^-} , and J_{tot} .

Generally, however, the electrochemical system is analysed by fixing one of the two variables, V or J_{tot} . Specifically, when V is fixed, the system operates under potentiostatic conditions, whereas when J_{tot} is fixed, it operates under galvanostatic conditions. In both cases, the resulting system of three equations with three unknowns is solvable.

The solutions of the system are, respectively, for the potentiostatic case:

$$\left\{ \begin{aligned} J_{\text{TOT}} &= - \frac{(R_{\text{CO}_3^-} + R_{\text{OH}^-}) * V - (E_{\text{OH}^-} * R_{\text{CO}_3^-} + E_{\text{CO}_3^-} * R_{\text{OH}^-})}{R_{\text{EXT}} * (R_{\text{CO}_3^-} + R_{\text{OH}^-}) + R_{\text{OH}^-} * R_{\text{CO}_3^-}} \end{aligned} \right. \quad \text{Equation 11}$$

$$\left\{ \begin{aligned} J_{\text{CO}_3^-} &= - \frac{R_{\text{OH}^-} * V - (E_{\text{OH}^-} - E_{\text{CO}_3^-}) * R_{\text{EXT}} - E_{\text{CO}_3^-} * R_{\text{OH}^-}}{R_{\text{EXT}} * (R_{\text{CO}_3^-} + R_{\text{OH}^-}) + R_{\text{OH}^-} * R_{\text{CO}_3^-}} \end{aligned} \right. \quad \text{Equation 12}$$

$$\left\{ \begin{aligned} J_{\text{OH}^-} &= - \frac{R_{\text{CO}_3^-} * V - (E_{\text{OH}^-} - E_{\text{CO}_3^-}) * R_{\text{EXT}} - E_{\text{OH}^-} * R_{\text{CO}_3^-}}{R_{\text{EXT}} * (R_{\text{CO}_3^-} + R_{\text{OH}^-}) + R_{\text{OH}^-} * R_{\text{CO}_3^-}} \end{aligned} \right. \quad \text{Equation 13}$$

And for the galvanostatic case:

$$\left\{ \begin{aligned} V &= - \frac{R_{\text{EXT}} (J_{\text{TOT}} * R_{\text{OH}^-} + J_{\text{TOT}} * R_{\text{CO}_3^-}) + R_{\text{CO}_3^-} * (J_{\text{TOT}} * R_{\text{OH}^-} - E_{\text{OH}^-}) + E_{\text{CO}_3^-} * R_{\text{OH}^-}}{R_{\text{CO}_3^-} + R_{\text{OH}^-}} \end{aligned} \right. \quad \text{Equation 14}$$

$$\left\{ \begin{aligned} J_{\text{CO}_3^-} &= \frac{J_{\text{TOT}} * R_{\text{OH}^-} - E_{\text{OH}^-} + E_{\text{CO}_3^-}}{R_{\text{CO}_3^-} + R_{\text{OH}^-}} \end{aligned} \right. \quad \text{Equation 15}$$

$$\left\{ \begin{aligned} J_{\text{OH}^-} &= \frac{J_{\text{TOT}} * R_{\text{CO}_3^-} - E_{\text{CO}_3^-} + E_{\text{OH}^-}}{R_{\text{CO}_3^-} + R_{\text{OH}^-}} \end{aligned} \right. \quad \text{Equation 16}$$

This kinetic model is then inserted into a model that allows a accurate prediction and simulation of the entire cell environment. Specifically, assuming the water–gas shift reaction is occurring at the anode and is at thermodynamic equilibrium, considering the diffusion of the reagents towards the electrode surface inside the cathodic compartment and based on Faraday’s law, macroscopic mass and energy balances are applied to calculate the cell outlet streams in terms of temperature and composition.

As far as specific cell parameters are concerned, a current density of 1000 A/m² has been used, coupled with a hydrogen utilisation of 75% and a CO₂ utilisation factor of 85% [135], [136]. The fitting parameters for the electrochemical kinetic were taken from previous works of the group, that were experimentally validated [137].

5.2 Open-source Chemical Process Simulator - DWSIM

The code was initially developed in FORTRAN for implementation within Aspen Plus, a commercial process simulation software widely used in industry for modelling and optimizing chemical processes. It was subsequently translated into Python for integration into DWSIM, an open-source, CAPE-OPEN compliant process simulator that enables flexible process modelling and is particularly suited for educational and research purposes. Adopting an open-source platform like DWSIM imposes no limitations on the distribution of the developed models, thereby supporting wider accessibility and fostering ongoing collaborative efforts.

5.3 System simulation

Approaching the simulation of a CCS system for on board carbon capture and storage, different parameters must be considered: cost, capture rate, energy efficiency, fuel efficiency and volumes. All these parameters have an important impact on the utility of the studied solutions and will be discussed in the results sections. The simulations consider exhaust gas streams from naval engines operating on different fuels, LNG that is represented as methane in the model for the purposes of the reforming reactions and burner fuel and finally steam is included as a utility stream, since it can be available both onboard and in shore-based plants. In addition, multiple CO₂ capture rates were evaluated to assess performance across different capture targets.

As far as CCS systems with MCFCs are concerned, in literature few such processes have been discussed, with the main one proposing two solutions, one that produces cell fuel (Hydrogen and CO) through a reforming reaction of LNG and separates the obtained carbon dioxide through liquefaction. The second solution still uses a reforming reaction but obtained separation through the usage of a membrane [138]. As is explained in the paper found during literature review, the introduction of the membrane does not improve the system significantly while also making it more complex, therefore the basic system has been considered as the starting point for the simulations and optimisations from here on.

Three big potential improvements have been studied and implemented inside the process simulation to increase the system overall efficiency and capture rate, those being:

- Introduction of recycles

- Changing type of reforming (SMR and DMR)
- Introduction of an electrically heated reforming reactor (eSMR)

5.3.1 Methane reforming overview

The steam methane reforming reaction is used today to produce around 50% of the hydrogen supply required globally and is a well-established technology [139], [140]. The steam methane reforming (SMR) reaction is an exothermic catalysed reaction that breaks down methane and higher hydrocarbons using steam as a co reactant to obtain carbon dioxide, carbon monoxide and hydrogen, a mixture usually known as Syn Gas. The reaction can happen in a wide range of temperature and pressure, as it depends on the chosen degree of conversion of the methane, but to obtain a high conversion of methane (>99%) as is of interest in this work a temperature range of around 700 – 1000°C is used [141], whilst a pressure of 30 – 40 bar is recommended [142], for the on board application and the compatibility of the gas pressure with the cell, the reaction will be kept at around atmospheric pressure which increases the volume of the process but reduces the overall system complexity [143].

The reactions for the SMR process are as follows:



The ratio between the water and carbon content determines the reaction equilibrium for the second reaction involved, being the Water Gas Shift (Reaction 11) that consumes part of the monoxide to increase the yield of carbon dioxide. This ratio, called Steam-to-Carbon, S/C, usually ranges between 2 and 4 [144], for the application in this case a starting ratio of around 4 has been chosen. This is because steam is also important to inhibit secondary reactions being the carbon deposition, which can happen at high temperatures in presence of dry carbon gas as follows:



The two reactions are respectively the decomposition of methane and the Boudouard Reaction (Reaction 13). In the CCS system it has been chosen to work at high steam to carbon to assure a sufficient steam content also in the gases inside the fuel cell, avoiding a carbon deposition inside the tubing and the MCFC itself [145].

Usually three reactors are used in the SMR process, namely, a pre reforming, a main reforming and a water gas shift reactor [146], to increase the selectivity towards hydrogen and decrease the content of CO, as monoxide is usually problematic inside fuel cell application at low temperatures [147]. In the case of MCFCs,

this is not the case, as the monoxide can be turned into more fuel inside the cell through the water gas shift reaction [148].

The dry methane reforming reaction is gaining traction as of recently, as it uses carbon dioxide as a co reactant instead of steam inside the reactor, meaning that it is possible to have a direct carbon dioxide utilisation [149].

This reaction as the steam methane reforming variant is a catalytic exothermic reaction, that usually is done at temperatures of 700 – 1300 °C and a pressure of 1 – 10 bar [150], and the reactions are as follows:



The conventional DMR process has a lower conversion of methane when compared to the SMR (>75% at 900°C [151]) while more unconventional reactor designs can also reach the same conversions (>99% [152]). For the means of this work a traditional and more proven design has been chosen, working at atmospheric pressure and a temperature around 900°C.

5.3.2 Steam Methane Reforming (SMR)

The first configuration examined corresponds to the most conventional approach, commonly referenced in the existing literature and can be seen in Figure 5-2. In this setup, the cathodic side (21), which is where the engine exhaust gases are fed, is initially preheated to 580 °C (22) before being fed into the fuel cell. Upon exiting the cell, the cathodic exhaust stream (23), now depleted in CO₂, is combined with the cooled anodic recycle stream (14) and a supply of liquefied natural gas (LNG) (15). This combined stream (16) is directed to a burner, which serves to provide the necessary heat input for the steam methane reforming (SMR) reactor, operating at 800 °C.

To ensure effective heat exchange, the burner temperature is maintained at 850 °C, following the design guideline that pose a minimum temperature difference of 50 °C between the inlet of the hot stream and the outlet of the cold stream. After the burner (17), the resulting hot gas is employed to preheat incoming process gases (17 + 18) before being discharged to the exhaust (19), here the stream is cooled down to the inlet temperature for heat recovery and sent to the chimney (20).

On the anodic side, the inlet mixture (3), made by a mixture of LNG (1) and steam (2), is similarly preheated to 800 °C using the high-temperature exhaust gases from the burner. A steam-to-carbon ration of 4:1 was used to ensure sufficient steam both for the SMR and to avoid carbon deposits in the cell afterwards [153]. This preheated stream is then introduced into the SMR unit (4), where methane is converted to syngas with a conversion efficiency exceeding 99%. The generated syngas (5) is subsequently mixed with recycled anodic gases and cooled to 580 °C prior to entering the fuel cell (6). This temperature moderation is critical for thermal management within the cell, given the exothermic nature of the electrochemical reactions, which necessitates active cooling. The mean temperature between the input and output temperature should be in the range of 650°C.

Following electrochemical conversion, the anodic exhaust (7), rich in carbon dioxide, is subjected to an initial cooling step. This is typically achieved using seawater, though the same thermal energy could alternatively be used to generate additional process steam, depending on the system's integration and steam requirements. Water is removed via condensation (9), and the remaining gas stream undergoes cryogenic separation to isolate high-purity liquid CO₂ (11).

The cleaned anode stream (12), composed primarily of unreacted fuel, is then divided: approximately 75% is recycled to the anodic inlet (13), while the remaining 25% (14) is routed to the burner along with the cathodic exhaust (22) and a supplemental LNG feed (15). This composition is calibrated to provide the thermal energy required by the SMR, based on an assumed heat transfer efficiency of 80%.

The electricity from the cell (E1) is divided into three contributions: one is the electricity required for the cryogenic separation (E3), the balance of plant (BOP) (E2) and the remainder is sent to the engines (E4).

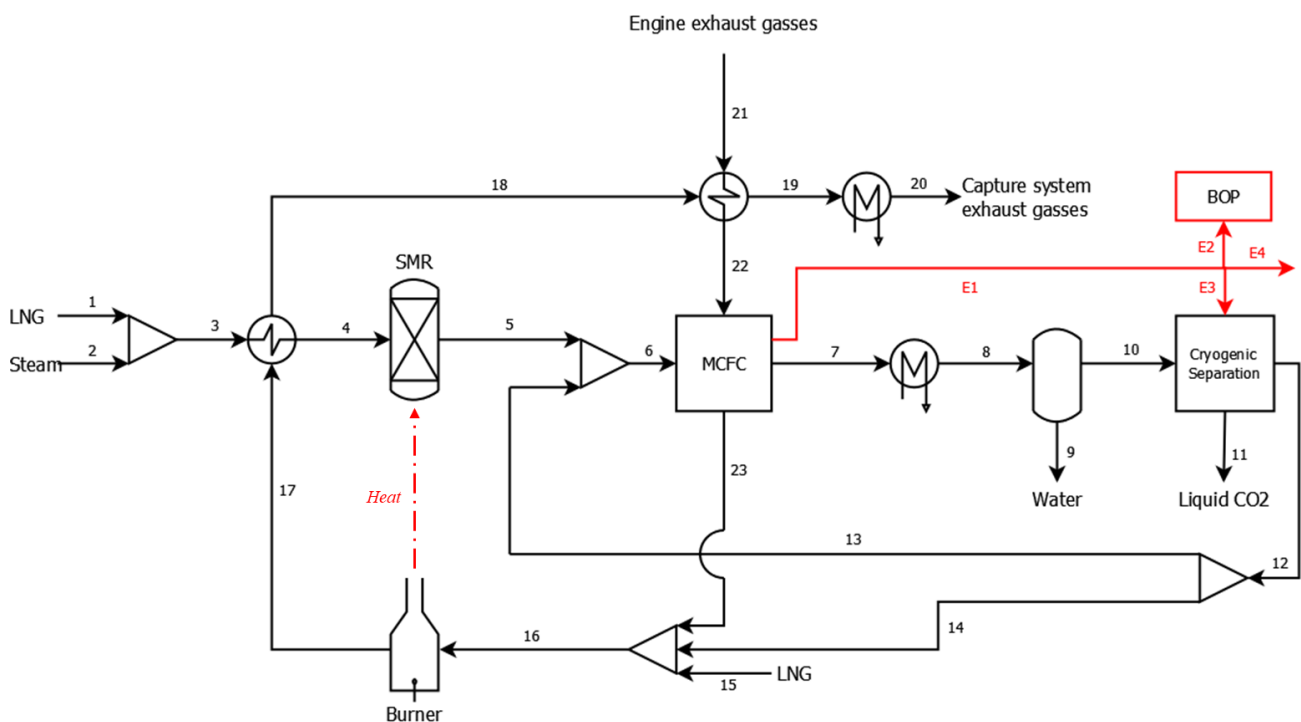


Figure 5-2 Carbon capture system based on traditional SMR technology without a recycle of the burner gases towards the cathodic input. The black streams refer to material streams, while the red ones are referred to energy streams.

5.3.3 Steam Methane Reforming (SMR) with recycle

The second system developed addresses a key limitation identified in the first configuration namely, the substantial production of carbon dioxide from the burner itself, which negatively affected the overall CO₂ capture rate. To mitigate this issue, the exhaust gases from the burner are redirected and recycled to the cathodic inlet stream as can be seen in Figure 5-3.

In this configuration, the cathodic feed gases (20) are initially blended with the hot combustion products from the burner (19). A subsequent preheating stage then raises the gas mixture (21) temperature to 580 °C via heat exchange with the cathodic exhaust gases exiting the fuel cell. The preheated gases (22) are then introduced

5.3.4 Dry Methane Reforming (DMR)

In this configuration seen in Figure 5-4, the system is modified to redirect a portion of the CO₂-rich anodic exhaust gas (10), post-condensation but prior to cryogenic CO₂ separation, toward the liquefied natural gas (LNG) feed stream.

On the cathodic side, the process mirrors the traditional approach: incoming carbon rich exhaust gases (23) are preheated using exhaust gases (20) from the burner and introduced into the fuel cell at 580 °C (24). The cleaned cathodic gas stream is then sent towards the burner to provide the necessary oxygen content for the combustion (25).

The anodic stream begins with a mixture of LNG (1) and recycled anodic gas (10). Since this recycled stream has already undergone water condensation but not CO₂ removal, it is rich in carbon dioxide. The mixture (2) is formulated to maintain a molar CO₂-to-LNG ratio of approximately 1:1.5 [154]. This combined stream is preheated (3) and introduced into the reforming reactor, where it undergoes dry reforming to produce a syngas composed primarily of hydrogen and carbon monoxide (4).

Following reforming, the syngas (4) is blended with a hydrogen-rich anodic recycle stream (14) and a controlled amount of steam (15). The addition of steam is essential to suppress carbon deposition within the fuel cell, as the presence of a hot, carbon-rich gas in the absence of sufficient steam poses a significant risk for coke formation. The steam is introduced at a molar ratio of S/C = 1.5:1 relative to the total carbonaceous species (CH₄, CO, and CO₂), as recommended by recent literature[155]. During operation, additional steam is generated internally through electrochemical oxidation and water-gas shift reactions, further enhancing the steam-to-carbon ratio and maintaining system stability.

Post-cell, the anodic exhaust stream (6) is initially cooled via seawater exchange (7), allowing for condensation of water (8). The cooled gas (9) is then partially recycled to the LNG inlet to sustain the required CO₂ concentration (10). The remaining portion is routed through a cryogenic separation unit to recover high-purity CO₂ (12). The residual anodic gas from this process is divided: approximately 25% is recycled back to the anode inlet (14), while the remainder is directed to the burner (16).

In the burner, this stream is combined with cathodic exhaust (24) and a supplemental supply of LNG (17) to supply the necessary thermal energy for the reforming reactor. The hot combustion gases (19) produced are then employed to preheat the incoming process gases before being vented to the exhaust (22) after a heat recovery (21).

The electricity from the cell (E1) is divided into three contributions: one is the electricity required for the cryogenic separation (E3), the balance of plant (BOP) (E2) and the remainder is sent to the engines (E4).

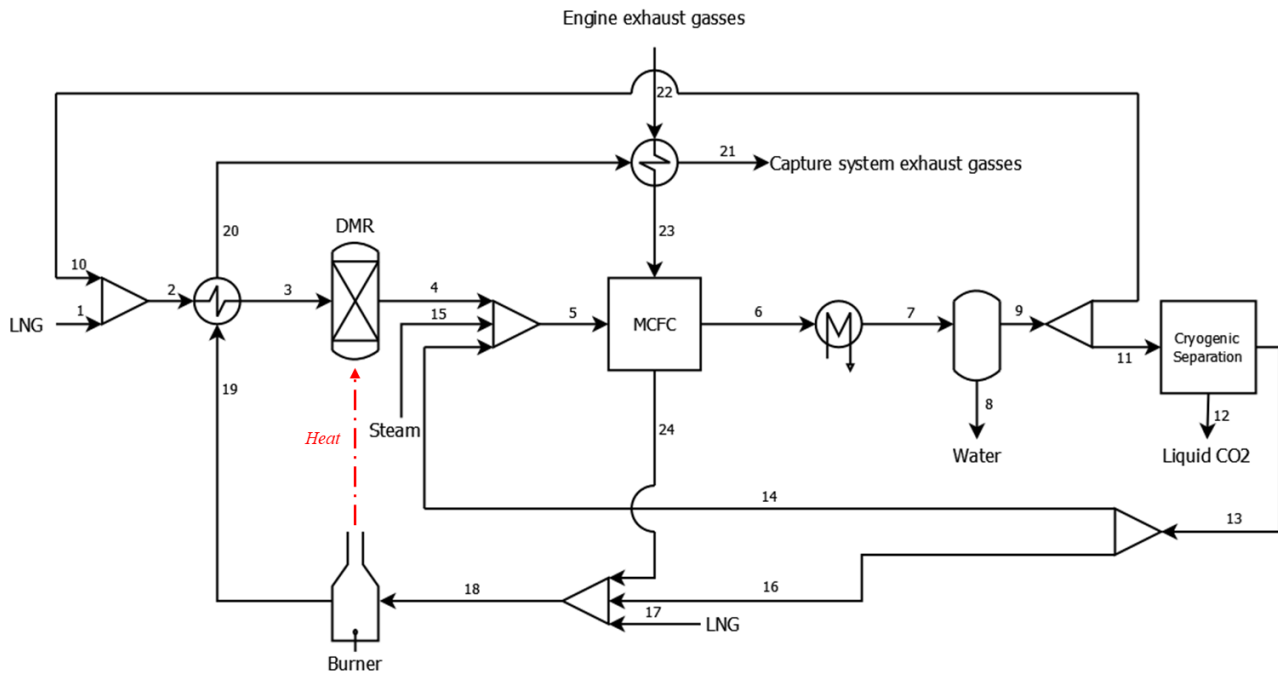


Figure 5-4 Carbon capture system based on DMR technology without a recycle of the burner gases towards the cathodic input. The black streams refer to material streams, while the red ones are referred to energy streams.

5.3.5 Dry Methane Reforming (DMR) with recycle

Given that carbon dioxide emissions from the burner were identified as a significant factor limiting the overall CO₂ capture rate in the traditional system, the dry methane reforming (DMR) configuration was also evaluated under similar optimization conditions. In this optimized DMR system, efforts were made to minimize the CO₂ contribution from combustion by adjusting the flow structure and integrating partial gas recycling as seen in Figure 5-5.

As observed in the steam methane reforming (SMR) configuration with recycle, the cathodic gas stream follows a simplified pathway. The cathodic gas (22), mixed with the recycle of gases from the burner (23), is preheated via heat exchange with the exiting cathodic exhaust (25), ensuring it enters the fuel cell at the target temperature of 580 °C (24). The cleaned cathodic gases are then sent for heat exchange towards the input of the cathodic gases and then to the exhaust. Before being released into the air, the gases are cooled down to the inlet temperature again (27).

The anodic side operates as in the DMR system without cathodic recycle. Initially, liquefied natural gas (LNG) (1) is mixed with a CO₂-rich recycled stream originating from the anodic exhaust (10), collected prior to cryogenic CO₂ separation but after water condensation. This mixture (2) is then heated (3) and sent to the DMR reactor, operating at 893 °C, where syngas formation occurs. Following reforming, the gas stream (4) is combined with steam (15) and a hydrogen-rich anodic recycle stream (14) before being introduced into the fuel cell at 580 °C.

After the electrochemical reaction in the cell, the anodic exhaust (6) undergoes a first cooling stage (7) to condense and separate water (8). A portion of the dry gas is recycled to the LNG input to sustain the desired CO₂/CH₄ ratio for DMR (10), while the remainder (11) is directed to a cryogenic separation unit for CO₂

removal (12). The resulting clean anodic gas stream is again split approximately 25% (14) is recycled back to the anode inlet, while the remaining 75% is sent to the burner (16).

As in the SMR system with recycle, the burner stream is supplemented with air to provide the oxygen required for complete combustion of the fuel components and LNG to supply the required thermal energy for the reforming reactor (17). The air is introduced at 20% more than the stoichiometric requirement to ensure sufficient oxygen availability for the combustion of LNG, hydrogen, and carbon monoxide (18). The hot exhaust gases (20) generated from this process are used to preheat the incoming anodic feed (2), after which they are directed to the cathodic inlet (21). This configuration enables further CO₂ capture from the burner exhaust by mixing the burner exhaust with the cathodic side input.

The electricity from the cell (E1) is divided into three contributions: one is the electricity required for the cryogenic separation (E3), the balance of plant (BOP) (E2) and the remainder is sent to the engines (E4).

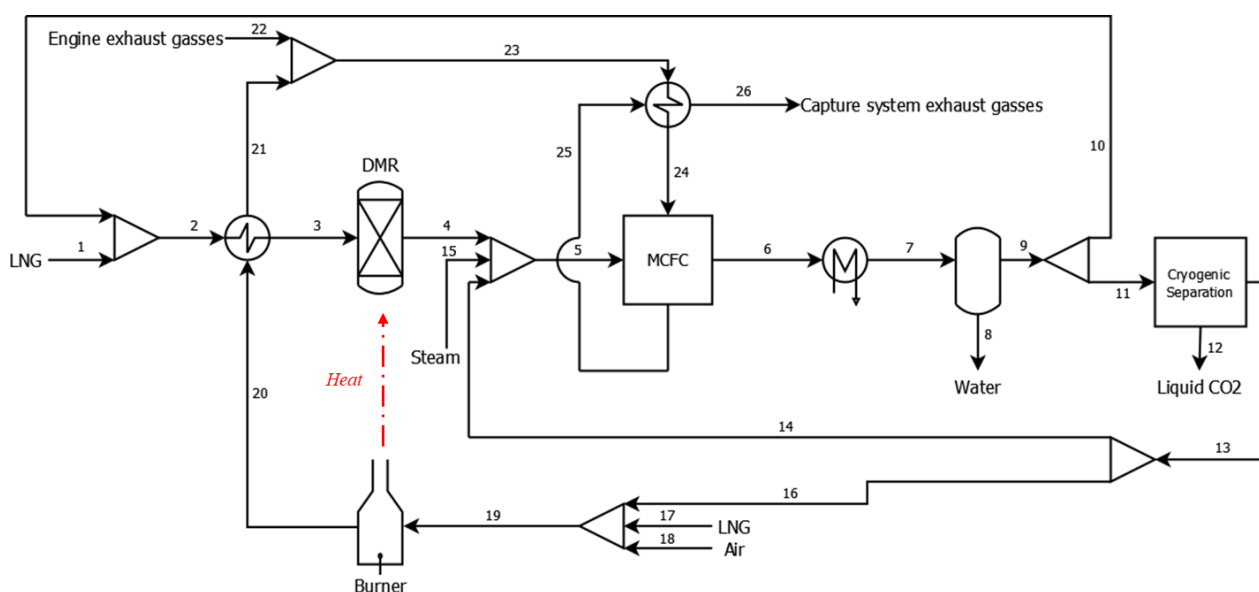


Figure 5-5 Carbon capture system based on DMR technology with a recycle of the burner gases towards the cathodic input. The black streams refer to material streams, while the red ones are referred to energy streams.

5.3.6 Electrical Steam methane reforming (eSMR)

One limitation of this system is the fact that while capturing CO₂, some is being produced for the heating of the reformer. While this issue is reduced by recycling the gases at the cathodic input, it is still overall decremental to the overall performance of the system. To address this issue, a recent development in SMR technology was adopted, namely an electrically heated reformer. This system, seen in Figure 5-6, has different advantages when compared to the traditional reformer. Firstly, the heating system being electrical removes the need for the burner. Secondly, the space requirements of the system decrease, as the burner can be removed, but also the footprint of the electrical reformer is significantly lower than the one of a traditional reformer [156]. Thirdly, one aspect that must be considered is that the power generated inside the MCFC fuel cell is in

direct current (DC), and inverter stations need to be inserted in the system overall volume balance to provide alternated current to the external environment. In this case part of the power of the cell can be used to heat the reformer which also requires direct current, decreasing the need for inverter volume [157].

The cathodic side of the system follows the same principle established in the previously discussed configurations employing cathodic recycle. In this arrangement, the cathodic gas stream is introduced into the system (15), preheated through heat exchange with the cathodic exhaust exiting the fuel cell (17), and brought to a temperature of 580 °C before being sent to the fuel cell (16). After the cell, the clean gas (17) is firstly used to heat up the cathodic input and then sent towards the gas exhaust (18).

On the anodic side, the feed consists of three components: liquefied natural gas (LNG) (1), steam (2), and a recycled portion of the anodic exhaust gases (14). The anodic recycle is introduced upstream of the reformer. This configuration is essential in the absence of a burner, since without combustion to consume residual methane, unconverted hydrocarbons could accumulate within the system. Positioning the recycle before the reformer ensures sufficient methane conversion and maintains the chemical stability of the process.

The resulting mixture is heated in two stages. Initially, it is brought to approximately 550 °C (3) using heat from the anodic exhaust gases from the cell (8). In the second stage (4), the hot effluent from the reformer (6) is used to further raise the temperature of the feed stream to around 750 °C. Although the reformer operates at 800 °C, no available stream in the system reaches that temperature; the final thermal input is therefore provided internally within the reactor through heat transfer.

After reforming (6), the syngas, consisting mainly of hydrogen and carbon monoxide, is introduced into the fuel cell at 580 °C (7). During cell operation, electrochemical reactions result in a CO₂-enriched exhaust. This stream is first cooled (10) to condense and remove water (11), followed by cryogenic separation to isolate high-purity carbon dioxide (13). The remaining clean gas is then returned to the beginning of the process (14), where it is mixed once again with LNG and steam, thus completing the cycle.

The electricity from the cell (E1) is divided into four contributions: the first one is for the eSMR reactor (E2), the second one is the electricity required for the cryogenic separation (E4), the third one is the balance of plant (BOP) (E3) and the remainder is sent to the engines (E5).

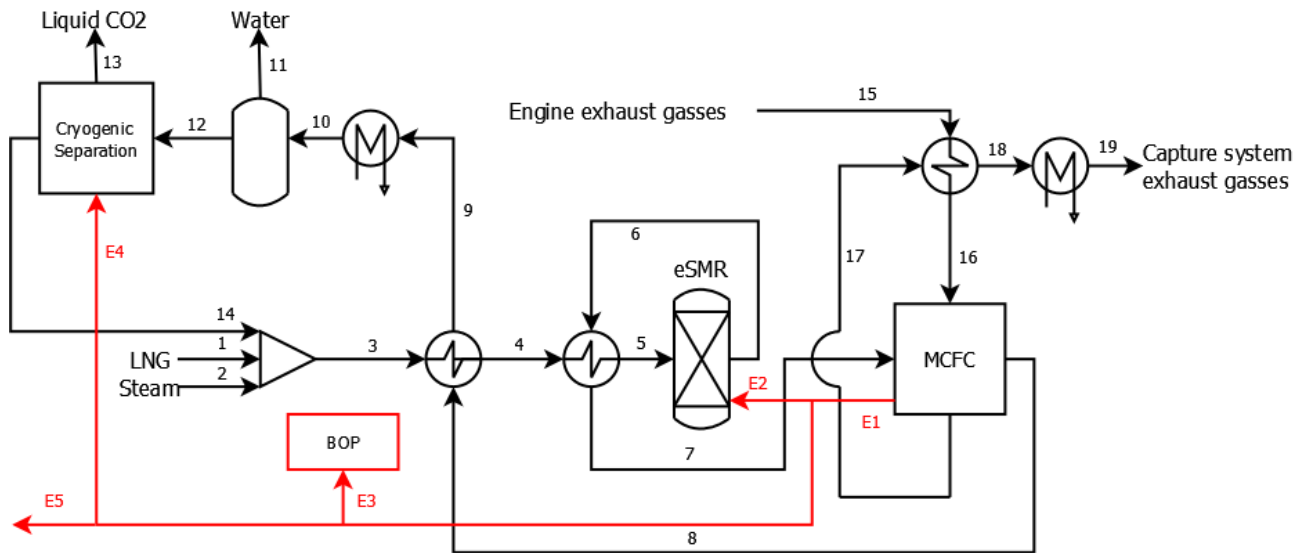


Figure 5-6 Carbon capture system based on SMR technology heated by electrical elements. The black streams refer to material streams, while the red ones are referred to energy streams.

5.3.7 System comparison

To evaluate these systems correctly some baselines had to be set, to provide consistency through all simulations. These overarching conditions were reassumed in Table 5-2.

*Table 5-2 Main simulation conditions, shared between the two case studies with LNG and HFO fuelled engine. *The electrical efficiency was set at 80% as a conservative assumption, reflecting the still low TRL of the eSMR technology. **Value from private communication from industrial partner. ***Conservative assumptions*

<i>Parameter</i>	<i>Value</i>
<i>Utilisation of hydrogen in the MCFC [158]</i>	75%
<i>Utilisation of CO₂ in the MCFC [158]</i>	85%
<i>Steam-to-carbon SMR [159]</i>	4:1
<i>CO₂-to-LNG DMR [160]</i>	1:1.5
<i>Temperature requirement between hot inlet temperature and cold outlet temperature</i>	+ 50°C***
<i>Burner SMR heat exchange efficiency</i>	80%***
<i>eSMR electrical heating efficiency</i>	80%*
<i>Auxiliary energy requirements</i>	10% of cell power***
<i>Liquefaction unit energy requirements</i>	0.2 MW/t _{CO2liquefied} **
<i>Power density cell [135], [161]</i>	0.1 A/cm ²

Furthermore, the power that the cell had in excess and that was therefore available for the vessel environment was considered to cover partially the energy requirements of the vessel generators. Doing so it is possible to reduce the power output of the engine and therefore the consumption of fuel. To do this correctly the SFOC of the vessel engines was considered to evaluate the non-linearity of consumption and engine load.

During the studies that have been conducted it was possible to note that the fuel type and engine SFOC could influence the system choice. To not favour a system purely based on the choice of the engine, two different engine have been considered, one fuelled with HFO and one with LNG. The main characteristics of these engines have been reported in the Table 5-3.

Table 5-3 Exhaust gas compositions, engine power at full load and gas emissions at full load of both the engines that have been studied in this thesis simulations.

Parameter	Engine type MAN 48/60 CR		Engine type Wärtsilä 34 DF	
	[162]		[163]	
Power [kW]	10800		8000	
Fuel	HFO		LNG	
Carbon factor	3.114		2.75	
Gas emissions at 100% load [kg/h]	77953		43567	
Temperature [°C]	361		360	
Exhaust gas composition [vol%]	CO ₂	5.2	CO ₂	4.4
	H ₂ O	5.4	H ₂ O	7.0
	O ₂	13.0	O ₂	12.0
	N ₂	76.4	N ₂	76.6

Finally, the last two inlet gases considered in the simulations were LNG (represented as pure methane in the model) and steam. The LNG stream was specified at 25 °C and 1 bar, whereas the steam stream was set to 144 °C and 4 atm. These operating conditions were derived from private communications with industrial partners and were adopted as representative and reasonable assumptions for onboard utility supplies.

The evaluation of the system performance was done considering different parameters, that are: fuel efficiency, cell dimension, thermal management, volume and system complexity.

All systems were evaluated against four net CO₂ capture targets: 20%, 40%, 60%, and 80%. As shown in the results, some configurations could not reach the full set of targets. For those systems, the analysis was therefore limited to the highest achievable capture level among the four specified targets. It is important to remember that the captured amount of CO₂ does not coincide with the amount of liquefied CO₂ as there is also a contribution by the amount of CO₂ that is being produced through the reforming reaction. Furthermore, the contribution of the cell to the engine allows the engine to operate at lower loads and this reduces the emissions further, increasing the net capture even more. The complete capture is evaluated as the CO₂ emissions of the

engine without the capture system compared to the system with the MCFC, therefore counting both the direct capture and the emission reduction.

5.3.7.1 Fuel consumption

The fuel consumption was evaluated considering the overall fuel usage, both for the reformer and the burner and then referred to the total captured CO₂, evaluated as difference between the input and the output to the capture system. For both HFO and LNG the burner was fed with LNG given it's lower carbon factor and the availability on board has to be granted for the reforming reaction in both cases.

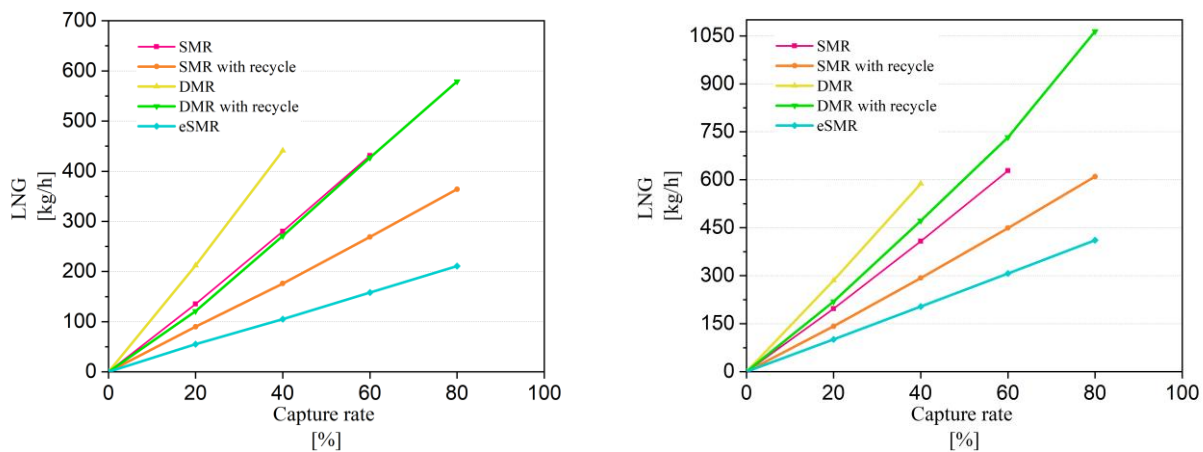


Figure 5-7 LNG consumption expressed in kg/h for all five studied system at different capture rates, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results

The overall fuel consumption for eSMR is the lowest for both cases and in all capture rates as evident in Figure 5-7, reaching 200 kg/h for the HFO capture and around 450 kg/h for the highest capture in the LNG fuelled engine. The main difference between the two graphs is the distance between the SMR and DMR with recycle system, where the two have similar consumptions in the HFO case, mostly overlapping, this changes for the LNG case, as the SMR is always lower for the considered capture rates. This can be caused by the lower CO₂ concentration and stronger effect of the SFOC of the engine, in particular, HFO has a higher SFOC that is generally favoured when considering the reduction of the engine load, compared to LNG which already starts with a lower SFOC. Both DMR and SMR feel these effects less as they have less recycled, while DMR with recycle is significantly more sensible to changes in the gas composition.

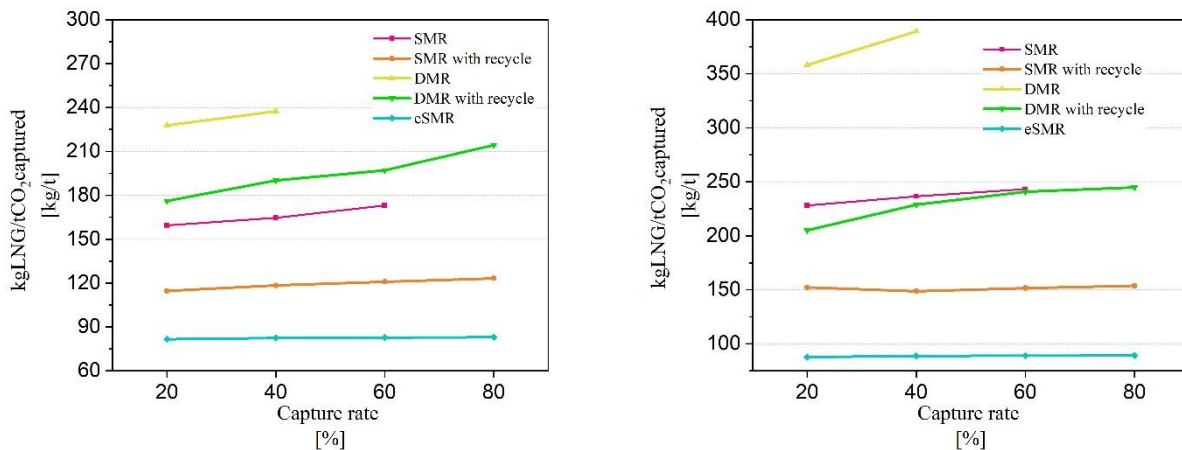


Figure 5-8 Specific fuel consumption evaluated as $\text{kgLNG/tCO}_2\text{captured}$ for the evaluated capture targets, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results

This evaluation of the HFO fuelled engine shows in Figure 5-8 how firstly neither the SMR nor DMR system can reach a net capture rate of 80%, in the case of the DMR even 60% was too ambitious. However, the introduction of the recycles allowed both systems to reach the highest target. DMR, as to be expected had the highest LNG consumption for captured t of liquid CO₂. This is not surprising as the LNG is fed in excess compared to the CO₂ that is being used as a reagent inside the DMR reactor and has a lower conversion compared to the SMR system. The recycle still showed a significant improvement between the two systems, as the DMR alone at its highest capture rate (40%) reached a value of 237 $\text{kgLNG/tCO}_2\text{captured}$, while for the same capture rate the DMR with recycle required significantly less LNG, 190 $\text{kgLNG/tCO}_2\text{captured}$, meaning a 20% decrease. A similar behaviour can also be seen between SMR and SMR with recycle as at its highest capture rate SMR reached 173 $\text{kgLNG/tCO}_2\text{captured}$ compared to the 121 $\text{kgLNG/tCO}_2\text{captured}$ of the SMR with recycle system, meaning a 30% decrease in LNG requirement. At the highest capture rate, the eSMR system clearly outperforms the alternatives, requiring 33% less LNG than the second-best configuration. (83 $\text{kgLNG/tCO}_2\text{captured}$ compared to 123 $\text{kgLNG/tCO}_2\text{captured}$ @80% capture rate).

As in the case of HFO, using LNG as the fuel neither SMR nor DMR were able to reach 80% net capture, with the latter not even reaching 60% net capture. The improvements of the recycle systems compared to their respective counterparts without recycle are higher than in the case of HFO fuelled engine. In this case, the SMR improves by 38% and DMR by 41% utilising the recycle of the gases (at the highest capture rate for the respective system). The eSMR system remains the best overall option, as in the previous case. That said, the capture process is more demanding for LNG-fuelled engine exhaust than for HFO exhaust, resulting in higher overall consumption across the board. This can stand by various factors amongst which the differing CO₂ concentration and consumptions under load of the two different engines. This also justifies the need to study these systems considering both options. In this case the eSMR system has a 41% reduced consumption compared to the second-best system in this field which is the SMR with recycle (89 $\text{kgLNG/tCO}_2\text{captured}$ compared to 154 $\text{kgLNG/tCO}_2\text{captured}$ @80% capture rate).

5.3.7.2 Cell active area

The cell active area of the MCFC needed for the operation of these CCS systems has been evaluated by evaluating the net cell power output and then specifically considering the cell number for captured unit of CO₂.

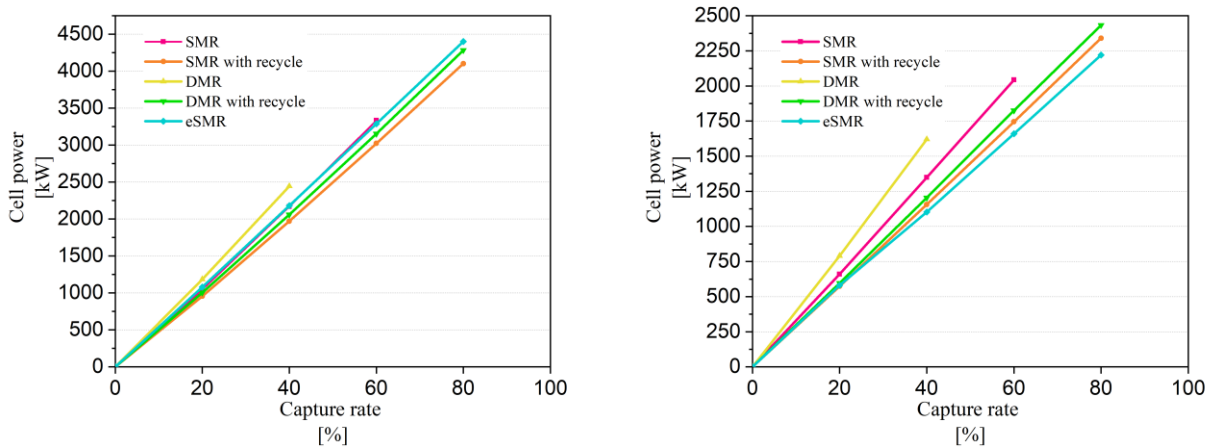


Figure 5-9 Cell power generation expressed in kW for all five studied system at different capture rates, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results

In the case of the cell power, the smaller the cell power required the better the ratio between required cell power and CO₂ capture. In this case, two different systems had the best performance depending on the case. In HFO, SMR with recycle has the least cell power output, while it is also true that the spread between all systems is very small in this case study. In the case of LNG, the eSMR system requires the least cell power, but the spread is visibly more accentuated. This could be caused again by the stronger SFOC and CO₂ concentrations. The fact that the cell is bigger for the systems without recycles could be because the lower concentration is not compensated by using recycles but stays lower throughout the whole process.

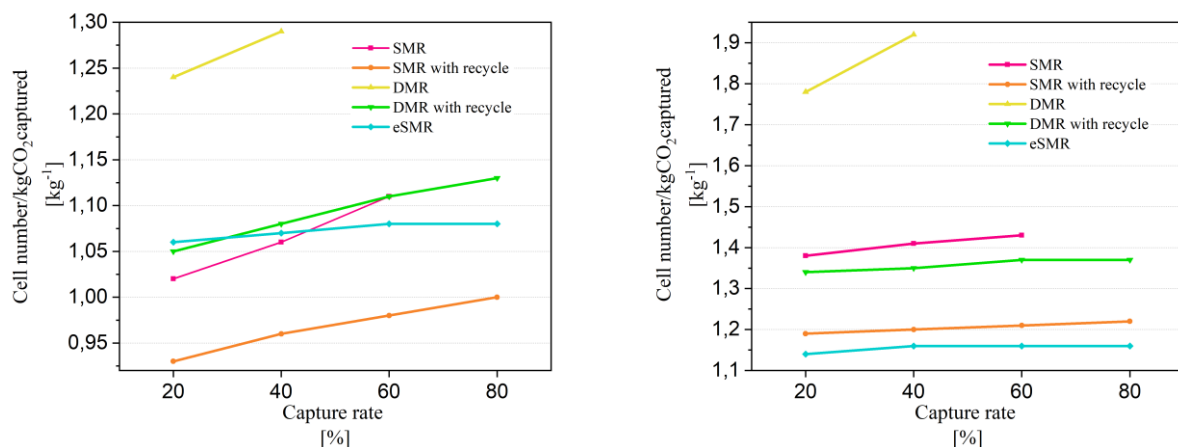


Figure 5-10 Specific cell active area evaluated as Cell number/kgCO₂captured for the evaluated capture targets, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results.

Looking at the specific cell active area for the HFO fuelled case as seen in Figure 5-10, SMR and DMR are both again the worst choices as they are not able to reach the highest capture rate requirements, but the improvements in terms of cell requirements by introducing the recycle is less noticeable compared to the fuel

consumption as SMR with recycle compared to SMR has a decrease of 12% of cells at the highest possible comparable capture rate (60%) while DMR with recycle compared to DMR has a reduction of cells of 16% (40% capture rate).

For the LNG case, the overall trend remains unchanged; however, the relative improvements provided by the recycle configuration and by eSMR become more pronounced. At a 60% capture rate, the base SMR configuration requires 17% more cells per captured unit than SMR with recycle. Similarly, the base DMR configuration requires 25% more cells than DMR with recycle. At the highest capture rate, eSMR requires 24% fewer cells than the second-best option (SMR with recycle). This suggests that in an LNG fuelled engine vessel the SMR could be the better option amongst the studied systems, even more as it already was in an HFO fuelled one.

The allocation of the cell power is usually distributed as follows: for conventional SMR, SMR with recycle, DMR, and DMR with recycle is assumed to be 10% to the balance of plant (BOP), 24% to liquefaction, and the remaining 66% to the engine. For eSMR, the split is different: 10% is allocated to the eSMR unit, 48% to the reactor, and 25% to liquefaction, leaving the remaining 17% for the engine.

5.3.7.3 Thermal management

Thermal management of the systems was analysed considering the net heat balance, therefore only counting the heat that is not required by the system itself as a heat output.

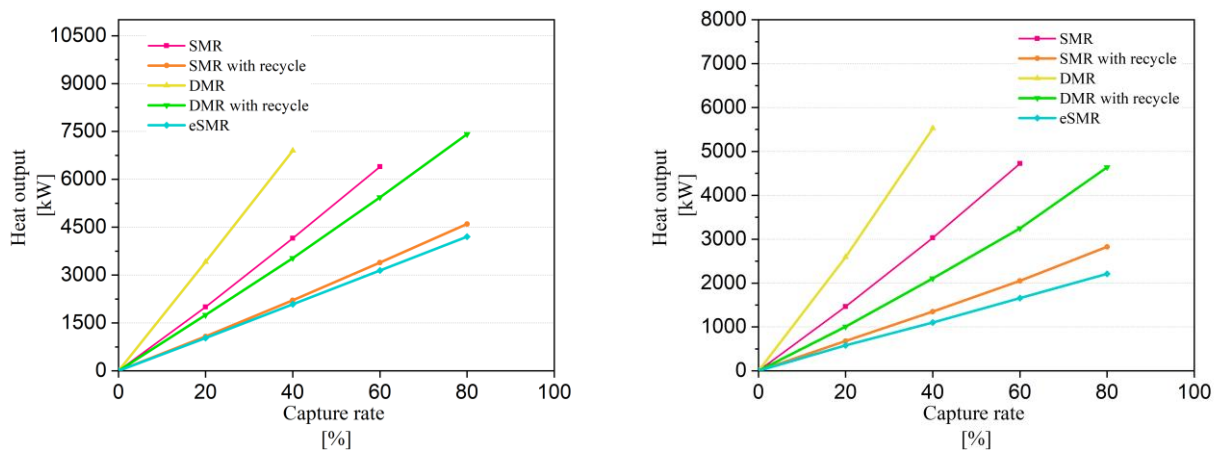


Figure 5-11 Net heat output expressed in kW for all five studied system at different capture rates, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results

In this case no significant difference between the trends of the two cases is notable looking at the graphs in Figure 5-11, although the spread in the LNG case study is again slightly larger than the one for HFO. eSMR and SMR have the lowest heat output of the analysed systems, while the systems without recycles have the highest, with DMR being markedly the highest. This is justifiable as the recycles help with thermal management by mixing hot and cold streams together, while without recycles the whole output of the burner is sent directly to the economiser after heat exchangers.

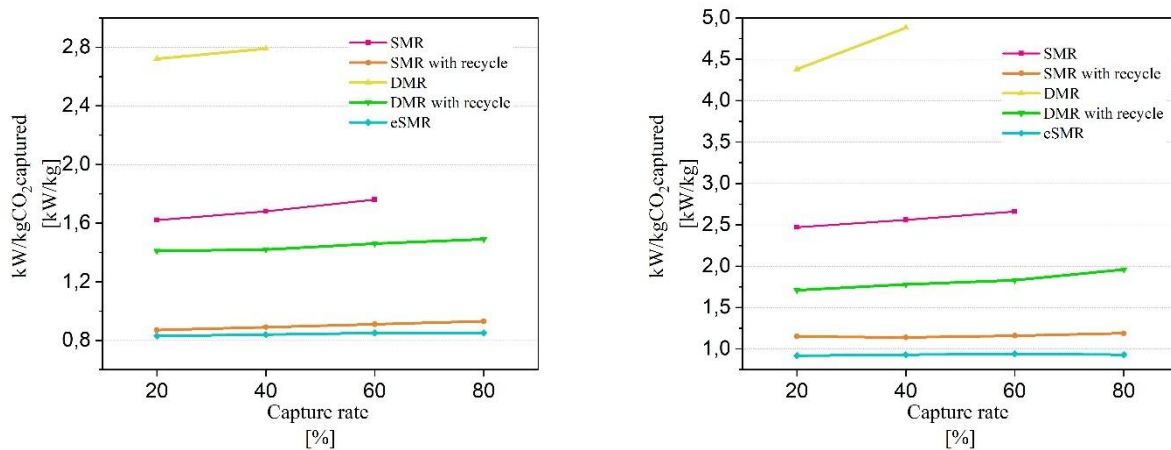


Figure 5-12 Specific heat output evaluated as kW/kgCO_2 captured for the evaluated capture targets, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results

Thermal management aspect is very important as it is a good indicator of the heat efficiency that the system can target and can be evaluated as seen in Figure 5-12. Having said this, depending on each application the heat output could be seen as a positive or as a negative aspect (i.e. steam generation for the vessel ecosystem). For both fuel types the eSMR system is the one with the least thermal dissipation, yet it is comparable with the SMR with recycle system. The DMR with recycle has a higher thermal output, also due to the necessity of working at higher temperatures in the reformer. The systems without recycle are the ones that have the least optimised heat management, as the absence of recycle of the cathodic gases causes a big loss in heat.

5.3.7.4 Volume

The volume evaluation has been performed on all systems as one of the most important parameters for on board applications is its compactness. To do this, some general guidelines have been used. The SMR and DMR reactors have been evaluated utilizing a typical residence time of these processes, while the eSMR reactor has been dimensioned knowing that it uses two orders of magnitude less volume than the traditional SMR reactor [70], [164], [165], [166]. For the heat exchangers a global heat exchange coefficient of $55 \text{ W/m}^2\text{K}$ and an exchanger compactness of $100 \text{ m}^2/\text{m}^3$ were adopted [167]. The cryogenic liquefaction units were found as a commercial solution and scaled depending on the flux of liquid CO_2 produced [168], [169]. The cell active area was scaled based on an internal preliminary engineering, coming out to around $22 \text{ m}^3/\text{MW}$. The excess electricity of the fuel cell, which is DC, will be transformed into AC using commercial inverter solutions [170]

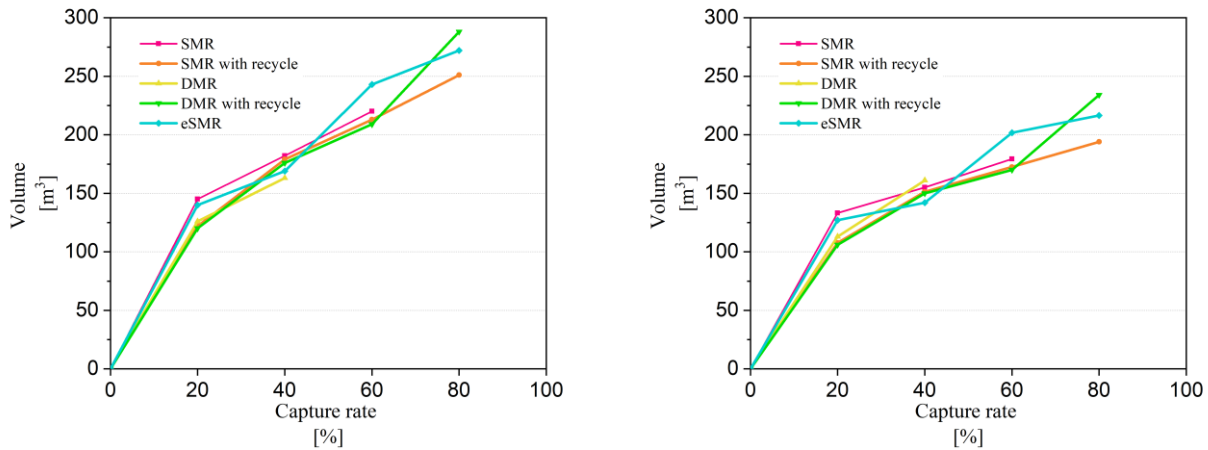


Figure 5-13 System footprint expressed in m^3 for all five studied system at different capture rates, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results

The volume trend can be seen in Figure 5-13 and it shows a non-linear behaviour which is partially caused by having chosen to use industrial “keys-in-hand” solutions for the dimensions. This allows the evaluation to be as realistic as possible, but obviously no solution will fit perfectly on the system’s needs, causing this interesting trend. Overall, the results indicate that increasing the capture rate tends to reduce the volume-related metric, with the rate of improvement diminishing at higher capture levels. Although no clear plateau is observed, the curves suggest that higher capture rates are generally more favourable in volumetric terms. A more robust comparison is therefore obtained by analysing the specific volume.

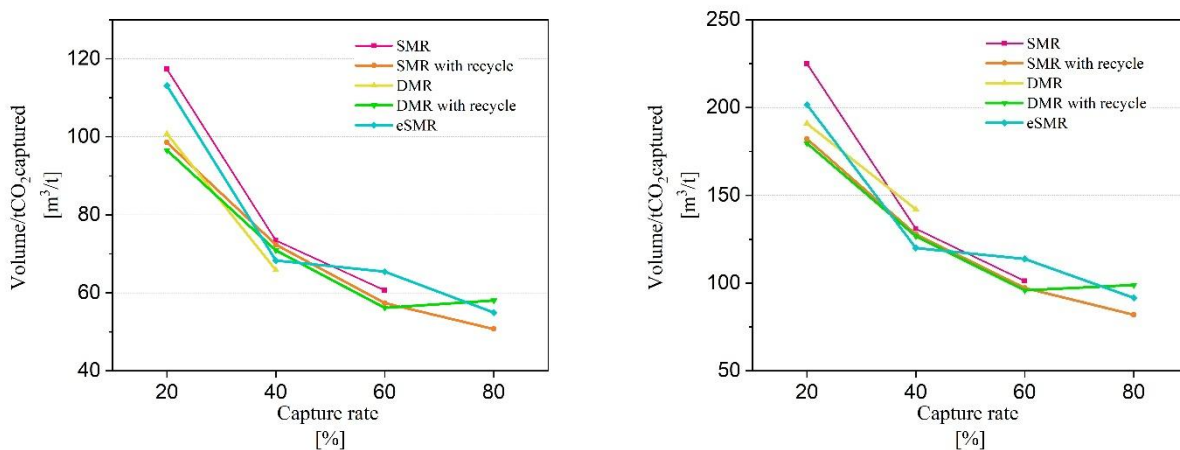


Figure 5-14 Specific volume evaluated as m^3/tCO_2 captured for the evaluated capture targets, in the left the HFO fuelled engine case study and on the right the LNG fuelled engine case study results.

The specific system volume is particularly interesting to analyse, as it highlights a clear non-linear relationship with the capture rates. This is largely because commercial solutions do not always align perfectly with the specific requirements of each system. In the case of the HFO fuelled engine the trend reveals that the three systems capable of achieving an 80% capture rate have very similar overall volumes, with each one proving to be the most suitable option for a particular capture target.

Looking at the LNG fuelled engine case, the non-linearity is even more acute; in the case of the DMR the specific volume has even a minimum at 60%, increasing again at 80%. Again, each of the three main solutions have an optimum capture case.

5.3.7.5 System complexity

The system complexity is not quantifiable like the parameters analysed before but requires a broader understanding of the system requirements in terms of know-how, operative phases and maintenance. A reduction of functional units relates to a reduction of complexity, and this shift is particularly evident when comparing SMR with recycle, DMR with recycle and eSMR. The first two system have a more complex layout, both requiring a burner not present in the eSMR and multiple split streams and recycles. The DMR also requires more know-how, as it is a less well-known process and therefore less specialised personal is available. It appears also evidently that both DMR and SMR without recycles are less complex than their evolutions with recycles. The trade-off however is the loss in overall capture rate.

Therefore, it is not possible to assign numerical values, however from these considerations a qualitative analysis can be done and represented as seen in graph.

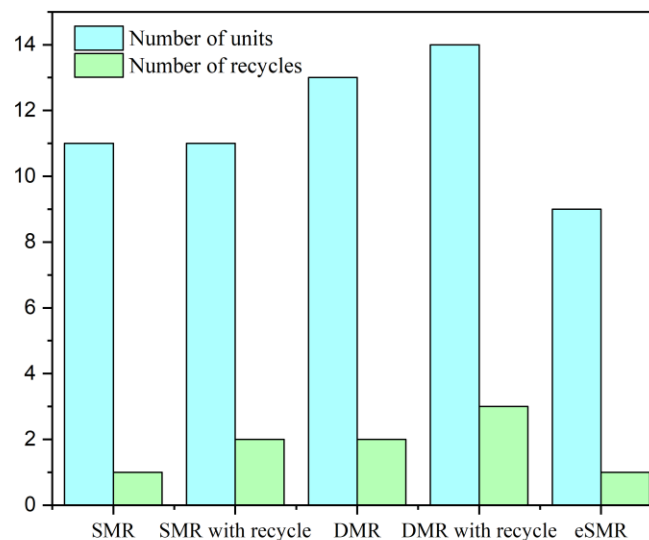


Figure 5-15 Number of units and recycles for all five studied system at different capture rates.

In this case, only the graphs in Figure 5-15 have been analysed as the systems do not change in terms of unit numbers between the different fuel options. The eSMR system has the lowest number of units (9) and is tied for the lowest amount of recycles (1), making it a potentially simple system. It is followed by the traditional SMR without recycles, with more units (11) but the same amount of recycles (1). Same number of units also for SMR with recycle (11), which adds one recycle to the count (2). The DMR without recycle has more units (13), tied for the second highest amount of recycles (2). And in last place is the DMR with recycles, which has 14 units and 3 recycles, making it the most complex system amongst the analysed. Furthermore, using a DMR

reaction implies also further knowhow as it is less common than SMR, which is the most used hydrogen production method.

5.3.7.6 OCCS system results

Having evaluated the main performance indicators of the systems, no clear best solution can be determined, yet it is possible to provide an overview of which system could be more favourable depending on the application case.

The main performance parameters for the systems can be summarised in Table 5-4. For the cell dimensions, the trend between HFO and LNG changes, in this case two values have been inserted to reflect this.

Table 5-4 A visual representation of the main results obtained for all analysed parameters. For the cell dimension, depending on the analysed case, both eSMR and SMR with recycle have been seen as the best solution, therefore this has been underlined by assigning two different votes to these depending on the case study, in brackets. The dots represent the affinity of the analysed system to the studied performance indicator; the more dots the system has the more it is aligned to the KPI.

	SMR	SMR with recycle	DMR	DMR with recycle	eSMR
<i>Fuel consumption</i>	●●●○○	●●●●○	●○○○○	●●○○○	●●●●●
<i>Cell active area</i>	●●●○○	●●●●●/●●●●○ (HFO/LNG)	●○○○○	●●○○○	●●●●●/●●●●● (HFO/LNG)
<i>Thermal management</i>	●●○○○	●●●●○	●○○○○	●●●○○	●●●●●
<i>Volume</i>	●○○○○	●●●●○	●●○○○	●●●○○	●●●●●
<i>System complexity</i>	●●●●○	●●○○○	●●●○○	●○○○○	●●●●●

As a closing statement, both eSMR and SMR with recycle are high potential solutions with similar performances, that have both strong and weak points compared to each other.

5.4 On land MCFC capture perspective

The systems that have been analysed before having been applied on a maritime vessel case, yet the necessity for carbon capture and carbon reduction is also present for on land application. In this case, the biggest contributions to the carbon emissions are from the industrial and energy sectors [171].

Within this PhD project, in collaboration with Duferco Engineering S.p.A., a case study was also carried out on the application of MCFC technology to a real industrial plant in Pallanzeno (Northern Italy), operated by Duferco Travi e Profilati S.p.A. The site covers over 400,000 m² and has a production capacity of around 675,000 tonnes per year. The plant is a hot-rolling facility specialized in long steel products, including the lamination of small- and medium-size HE and IPE beams, UPN and IPN profiles, equal and unequal angles, and special profiles (including earth-moving profiles) [172]. In this case, the sector is the one of steel manufacturing, which is responsible for 7% of the global CO₂ emissions [173].

The target was to find an option that was able to provide the highest possible capture rate. A limitation in the case of the analysed plant is that cathodic feed was very poor in oxygen as seen in Table 5-5, which can cause issues to the correct functioning of the cell as it is itself a reagent for the cathodic gas reaction. Therefore, an additional air stream is mixed in with the exhaust gases to achieve a target O₂ concentration of 10 vol%. Optionally, oxygen can also be provided as a pure stream, reducing the gas volumes as this avoids nitrogen additions as present in air.

Table 5-5 Composition of the exhaust gases, temperatures and gas flow of the gas emissions of a steel plant pre heating furnace.

<i>Gas emissions [Nm³/h]</i>	40000	
<i>Temperature [°C]</i>	430	
<i>Exhaust gas composition [vol%]</i>	CO ₂	9.2
	H ₂ O	17.9
	O ₂	0.9
	N ₂	72.0

The last two inlet gases considered in the simulations were LNG (represented as pure methane in the model) and steam. The LNG stream was specified at 25 °C and 1 bar, whereas the steam stream was set to 144 °C and 4 atm, in analogy with the on-board study.

Two solutions were studied in this case, one using a similar principle as the one seen in the previous study based on an eSMR reactor and one using an electrolyser to provide the hydrogen and oxygen.

5.4.1 eSMR

The first plant examined is like the one analysed for on-board-applications, as discussed in the previous chapter. The key difference that can be seen looking at Figure 5-16 lies in the addition of air (stream 16) to the engine exhaust gases (stream 15), which have a low oxygen content. This step increases the oxygen level in the resulting mixture (stream 17), bringing it up to 10%.

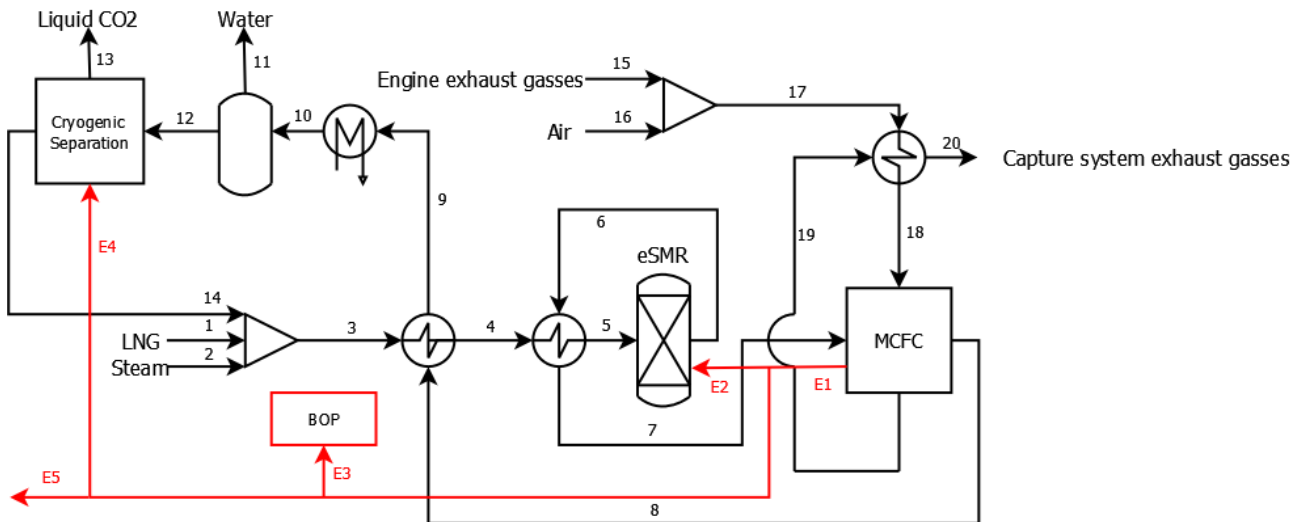


Figure 5-16 Carbon capture system based on SMR technology heated by electrical elements. An additional air stream is injected into the engine exhaust gases to allow to reach the desired oxygen concentration. The black streams refer to material streams, while the red ones are referred to energy streams.

5.4.2 Electrolyser MCFC

This process introduces a different way compared to the previous case studies to produce the fuel for the cell. While the previous applications had different layouts, all produced the fuel through a reforming reaction of natural gas, in this case, an electrolyser has been introduced as seen in Figure 5-17. This is usually not done because of the low energy efficiency but in this case the oxygen that is being produced by the electrolyser can be used to mix it with input gases to the cathode in order to increase the concentration of oxygen inside the stream, while avoiding the need to provide too much air, potentially compensating for the lower energy efficiency.

The anodic side has a feed of water (1) that goes inside the electrolyser, where it produces hydrogen (2) and oxygen (15). The hydrogen is then sent towards a mixer, here four streams mix, hydrogen (2), recycled hydrogen (13), steam (14) as it is required to avoid the carbon deposition inside the cell (as seen through the Boudouard reaction and then a CO₂ rich stream (10). The CO₂ rich stream is used to avoid the fast evaporation of the electrolyte inside the cell [174]. Before entering the cell, the mixture (3) is heated up with the stream coming from the fuel cell up to 580°C (4). After the cell, the stream is first used to heat up the incoming gases, the cooled down (7) to condensate water (8). The remainder is separated, one part is still rich in CO₂ and sent to the mixer (19), the other part is sent to the cryogenic separation (11), used to liquefy the CO₂ (12). The stream is then recycled back again towards the mixer as it is still rich in hydrogen.

The electricity from the cell (E1) is divided three contributions, part to the cryogenic separation unit (E2), part to the BOP (E4) and the remainder to the electrolyser (E3).

Table 5-6 Main results for the analysed case studies using the two mentioned systems at peak capture rate.

	eSMR	Electrolyser
<i>CO₂ capture rate [%]</i>	85.0	85.0
<i>Fuel consumption [kg_{LNG}/t_{CO₂captured}]</i>	95.0	116.0
<i>Cell power [MW/t_{CO₂captured}]</i>	1.0	1.1
<i>Volume [m³/t_{CO₂captured}]</i>	54.0	123.0
<i>Simplicity</i>	●●●○○	●●●●○

Both systems show a potentially high capture rate around 85%, making them both attractive under this viewpoint. They also show a very similar cell requirement of around 1 MW/t_{CO₂captured} of cell power. The main difference is found in terms of fuel demands, where the requirement of the electrolyser system has been evaluated by seeing the electrical power requirements and converting this requirement in equivalent LNG usage to be able to compare it with the eSMR system. Here the electrolyser system is much less competitive compared to eSMR. This is mainly because the electrolyser is, as mentioned before, not very energy efficient and it is not possible to cover the whole energy requirement by using the MCFC output (The electrolyser requires 15.47 MWh electricity input while the MCFC net output after covering all the balance of plant utilities and liquefaction is 4.75 MWh). This also means that one of the main advantages of the MCFC system, being its low energy requirement, is lost using the electrolyser system.

Furthermore, the eSMR system is more compact compared to the electrolyser system, this is mainly related to the fact that the electrolyzers require much bigger volumes compare to the reforming reactor, especially comparing it to the electrified version of it.

This comparison shows therefore, that while both systems are comparable in terms of capture efficiency, the electrolyser system cannot compete with the eSMR system as of now primarily because of the low energy efficiency of the electrolyser when compared to the reforming reaction to produce the hydrogen. The volume advantage of using pure oxygen to increase the oxygen content in the cathode is offset by the high volumes required by the electrolyzers and therefore the eSMR system using air for oxygen is still smaller.

6 Conclusions

Through the research done in this PhD project it was possible to determine that the MCFC technology has potential to allow for maritime sector decarbonisation. Furthermore, it was also demonstrated that utilising greener alternatives for part of the production process does not compromise the overall performance.

The MCFC produced with homemade matrix were able to reach performances of over 200 mW/cm², while also removing one of the compounds of greatest concern for human health and the environment present in the original recipes. Cell testing demonstrated that this performance was replicable, both with the same electrodes but also using other electrodes for both anodic and cathodic compartments. Testing of the components also in different gas conditions and temperatures has been done to evaluate the cell operational behaviour and confirm the good performance of the matrix.

System simulation showed that the CCS capability of the MCFC in a dedicated environment was able to reach competitive performance on-board thanks to different optimisation choices, being able to reach capture targets around 80% while only requiring an input of LNG and reducing the load of the studied engines thanks to its energy output. This can be particularly interesting when coupled with an LNG fuelled vessel as there is already the infrastructure present to handle this fuel, but it also had promising performance when coupled with an HFO fuelled engine.

For the best-performing configuration under each KPI, the main results indicate an LNG consumption of 83 kgLNG/t_{CO₂captured} for the HFO case and 89 kgLNG/t_{CO₂captured} for the LNG case, a required specific cell active area of approximately 1.0 (HFO) and 1.1 (LNG), and a heat output of 0.9 kW/kg_{CO₂captured} (HFO) and 1.0 kW/kg_{CO₂captured} (LNG). Overall system complexity varies with the selected solution, while the required specific volume decreases as the capture rate increases.

Thanks to a study also for on land applications, it was possible to determine that the technology can have promising performance for CCS also outside of the on-board utilization.

The main contributions of this thesis to research on this topic are:

- Development of a competitive MCFC matrix while eliminating the use of harmful solvents.
- Establishment of a new research environment at the Caplab facility, including the set-up of the required experimental infrastructure and procedures.
- Development and optimisation of an MCFC-based carbon capture system to separate CO₂ from exhaust gases, considering multiple fuel types and both on-land and on-board applications.

The next steps should focus on improving the production processes for the remaining cell components, starting with the electrodes. In addition, long-term testing is necessary to demonstrate the stability and durability of the developed materials under relevant operating conditions. Finally, the development of a pilot-scale MCFC-based CCS unit would enable validation of the simulation results and provide experimental data to further calibrate and optimise the model.

7 Papers and conferences

F.R. Bianchi, R. Risso , L. Cardona, D. Bove, F. Cannizzaro, L. Bonardi, E. Palmisani, B. Bosio; <i>Feasibility analysis of e-Hydrogen, e-Ammonia and e-Methanol synthesis compared with methane to fuel production</i> ; Fuel, 2025, https://doi.org/10.1016/j.fuel.2024.133938
R. Risso , D. Bove, B. Bosio; <i>Comparative analysis of different on-board CCS molten carbonate fuel cell solutions for IMO compliance</i> ; Greenhouse Gases: Science and Technology; 2025, https://doi.org/10.1002/ghg.70011
L. Cardona, R. Risso , J.P. P. Trujillo, D. Bove, C. Lagergren, B. Bosio; <i>New matrix improvement in MCFC applications</i> ; Under review 2025
L. Cardona, R. Risso , D. Bove, J.P. P. Trujillo, C. Lagergren, B. Bosio; <i>Matrix comparison in Molten Carbonate Fuel Cell application</i> ; International Congress on Sustainable Energy and related Technologies ICSET 2025
D. Bove, R. Risso , S. Formentini, D. Garibaldi, B. Bosio; <i>Fuel comparison for maritime Molten Carbonate Fuel Cell-integrated CO₂ capture systems</i> ; 5th September 2025 NEST Conference
L. Cardona, R. Risso , K. Hasanpour, M. Prati, D. Bove, B. Bosio; <i>Improvements in Matrix and Electrode Fabrication for Molten Carbonate Fuel Cell applications</i> ; 4th September 2025 NEST Conference
B. Bosio, F. Bianchi, R. Risso , L. Cardona, K. Hasanpour, M. Prati, D. Bove; <i>Material and Process Innovations for High-Performance MCFC Technologies</i> ; 14 – 17th September 2025 GRICU Congress
D. Bove, F. Bianchi, R. Risso , B. Bosio; <i>Evaluation of fuel options for marine MCFC-integrated carbon capture systems</i> , 14 – 17th September 2025, Poster at GRICU Congress
R. Risso , D. Bove, B. Bosio; <i>Molten carbonate fuel cells for carbon capture in steel sector</i> ; 17 – 19th September 2025, Oral presentation at European Fuel Cells and Hydrogen Conference 2025 (EFC 25)
F. Bianchi, D. Bove, L. Cardona, R. Risso , B. Bosio; <i>Feasibility analysis of green ammonia production based on solid oxide electrolysis cell technology</i> , 13th-15th September 2023, European Fuel Cells and Hydrogen Conference 2023 (EFC23)
M. Archetti, F. Bianchi, B. Bosio, D. Bove, I. Capestro, L. Cardona, R. Risso ; <i>CapLab: Electrochemical Cells</i> , 13th-15th September 2023, European Fuel Cells and Hydrogen Conference 2023 (EFC23)
L. Cardona, D. Bove, R. Risso , J.F. Basbus, M. Archetti, B. Bosio; <i>Development of matrices for Molten Carbonate Fuel Cells</i> , 13th-15th September 2023. European Fuel Cells and Hydrogen Conference 2023 (EFC23)
R. Risso , L. Cardona, M. Archetti, F. Lossani, B. Bosio, D. Bove; <i>A Review of On-Board Carbon Capture and Storage Techniques: Solutions to the 2030 IMO Regulations</i> , Energies 2023 16, 6748; https://doi.org/10.3390/en16186748
D. Bove, R. Risso , B. Bosio; <i>Feasibility analysis and design optimization of MCFC gas recirculation for enhanced carbon capture</i> , 4th Edition of International Conference on Green Chemistry and Renewable Energy 2024

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9 Appendix

9.1 SMR – HFO

Table 9-1 SMR; Fuelled with HFO; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	E1	E2	E3	E4
T	C	25	144	114	800	800	580	673	30	30	30	-30	-30	-30	-30	25	657	850	795	570	361	361	580	673				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,11	0,48	0,59	0,59	0,59	0,74	2,16	2,16	0,69	1,47	1,26	0,21	0,16	0,05	0,09	13,97	13,97	13,97	13,97	13,97	15,24	15,24	13,82				
Molar Flow	kmol/h	6,65	26,59	33,24	33,24	46,52	55,70	79,29	79,29	38,12	41,17	28,93	12,24	9,18	3,06	5,60	501,78	500,62	500,62	500,62	500,62	528,50	528,50	493,11				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,01	0,02	0,02	0,02	0,02	0,05	0,05	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,31	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,06	0,08	0,08	0,08	0,08	0,05	0,05	0,06				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,81	0,81	0,81	0,81	0,81	0,76	0,76	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,09	0,09	0,09	0,09	0,13	0,13	0,12				
Power	MWh																								1,04	0,10	0,24	0,69

Table 9-2 SMR; Fuelled with HFO; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	E1	E2	E3	E4
T	C	25	144	114	800	800	580	673	30	30	30	-30	-30	-30	-30	25	657	850	795	570	361	361	580	673				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,22	1,00	1,22	1,22	1,22	1,55	4,48	4,48	1,43	3,05	2,61	0,44	0,33	0,11	0,19	29,00	29,00	29,00	29,00	29,00	31,63	31,63	28,70				
Molar Flow	kmol/h	13,80	55,21	69,02	69,02	96,60	115,65	164,64	164,64	79,14	85,49	60,07	25,42	19,06	6,36	11,63	1041,85	1039,45	1039,45	1039,45	1039,45	1097,34	1097,34	1023,86				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,01	0,02	0,02	0,02	0,02	0,05	0,05	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,31	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,06	0,08	0,08	0,08	0,08	0,05	0,05	0,06				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,81	0,81	0,81	0,81	0,81	0,76	0,76	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,09	0,09	0,09	0,09	0,13	0,13	0,12				
Power	MWh																								2,17	0,22	0,51	1,44

Table 9-3 SMR; Fuelled with HFO; 60% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	E1	E2	E3	E4
T	C	25	144	114	800	800	580	673	30	30	30	-30	-30	-30	-30	25	657	850	795	570	361	361	580	673				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,34	1,53	1,87	1,87	1,87	2,38	6,89	6,89	2,19	4,69	4,02	0,67	0,51	0,17	0,29	44,62	44,62	44,62	44,62	44,62	48,67	48,67	44,17				
Molar Flow	kmol/h	21,24	84,96	106,19	106,19	148,63	177,97	253,33	253,33	121,78	131,56	92,43	39,13	29,34	9,78	17,90	1603,05	1599,35	1599,35	1599,35	1599,35	1688,42	1688,42	1575,37				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,01	0,02	0,02	0,02	0,02	0,05	0,05	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,31	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,06	0,08	0,08	0,08	0,08	0,05	0,05	0,06				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,81	0,81	0,81	0,81	0,81	0,76	0,76	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,09	0,09	0,09	0,09	0,13	0,13	0,12				
Power	MWh																								3,34	0,33	0,79	2,21

9.2 SMR with recycle – HFO

Table 9-4 SMR with recycle; Fuelled with HFO; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	678	30	30	30	-30	-30	10	10	25	25	21	850	250	361	350	580	678	428	361				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,10	0,44	0,54	0,54	0,54	0,68	1,97	1,97	0,63	1,34	1,15	0,20	0,15	0,05	0,04	1,09	1,18	1,18	1,18	11,78	12,96	12,96	11,67	11,67	11,67				
Molar Flow	kmol/h	6,09	24,36	30,44	30,44	42,61	51,15	72,69	72,69	34,90	37,79	26,40	11,39	8,55	2,85	2,75	37,67	43,27	42,18	42,18	408,55	450,73	450,73	418,43	418,43	418,43				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,08	0,02	0,20	0,20	0,20	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,00	0,02	0,09	0,09	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,06	0,06	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,76	0,76	0,76	0,82	0,82	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,13	0,12	0,12	0,10	0,10	0,10				
Power	MWh																										0,95	0,1	0,22	0,63

Table 9-5 SMR with recycle; Fuelled with HFO; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	678	30	30	30	-30	-30	-30	-30	25	25	21	850	250	361	350	580	678	428	361				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,20	0,91	1,11	1,11	1,11	1,41	4,07	4,07	1,30	2,77	2,37	0,40	0,30	0,10	0,09	2,24	2,43	2,43	2,43	24,30	26,73	26,73	24,07	24,07	24,07				
Molar Flow	kmol/h	12,56	50,24	62,80	62,80	87,90	105,50	149,94	149,94	72,01	77,94	54,47	23,47	17,60	5,87	5,68	77,68	89,22	86,99	86,99	842,84	929,83	929,83	863,16	863,16	863,16				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,08	0,02	0,20	0,20	0,20	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,00	0,02	0,09	0,09	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,06	0,06	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,76	0,76	0,76	0,82	0,82	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,13	0,12	0,12	0,10	0,10	0,10				
Power	MWh																										1,97	0,2	0,47	1,31

Table 9-6 SMR with recycle; Fuelled with HFO; 60% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	678	30	30	30	-30	-30	-30	-30	25	25	21	850	250	361	350	580	678	428	361				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,31	1,39	1,70	1,70	1,70	2,16	6,24	6,24	1,99	4,25	3,63	0,62	0,46	0,15	0,14	3,44	3,73	3,73	3,73	37,28	41,01	41,01	36,93	36,93	36,93				
Molar Flow	kmol/h	19,27	77,09	96,36	96,36	134,86	161,89	230,07	230,07	110,47	119,60	83,55	36,05	27,04	9,01	8,72	119,21	136,94	133,50	133,50	1293,11	1426,61	1426,61	1324,35	1324,35	1324,35				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,08	0,02	0,20	0,20	0,20	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,00	0,02	0,09	0,09	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,06	0,06	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,76	0,76	0,76	0,82	0,82	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,13	0,12	0,12	0,10	0,10	0,10				
Power	MWh																										3,02	0,3	0,71	2,01

Table 9-7 SMR with recycle; Fuelled with HFO; 80% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	678	30	30	30	-30	-30	-30	-30	25	25	21	850	250	361	350	580	678	428	361				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,42	1,89	2,30	2,30	2,30	2,93	8,47	8,47	2,70	5,77	4,93	0,84	0,63	0,21	0,19	4,67	5,07	5,07	5,07	50,59	55,66	55,66	50,12	50,12	50,12				
Molar Flow	kmol/h	26,15	104,61	130,76	130,76	183,01	219,71	312,22	312,22	149,91	162,31	113,39	48,93	36,69	12,23	11,83	161,78	185,84	181,18	181,18	1754,87	1936,05	1936,05	1797,27	1797,27	1797,27				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,08	0,02	0,20	0,20	0,20	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,00	0,02	0,09	0,09	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,56	0,56	0,56	0,00	0,00	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,06	0,06	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,76	0,76	0,76	0,82	0,82	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,13	0,12	0,12	0,10	0,10	0,10				
Power	MWh																										4,10	0,41	0,97	2,72

9.3 DMR – HFO

Table 9-8 DMR; Fuelled with HFO; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	27	893	893	580	696	30	30	30	30	30	-30	-30	10	150	-30	25	671	943	893	677	361	361	580	696				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,20	0,60	0,60	0,60	1,35	3,08	3,08	0,93	2,15	0,40	1,75	1,46	0,29	0,07	0,68	0,22	0,09	17,21	17,21	17,21	17,21	17,21	18,63	18,63	16,91				
Molar Flow	kmol/h	12,44	23,36	23,36	40,01	81,27	110,14	110,14	51,46	58,68	10,92	47,77	33,49	14,28	3,57	37,69	10,71	5,30	619,04	617,04	617,04	617,04	617,04	646,34	646,34	603,04				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,38	0,38	0,00	0,38	1,00	0,02	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,01	0,03	0,03	0,03	0,03	0,05	0,05	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,27	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	0,00	0,00	0,00	0,46	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,06	0,09	0,09	0,09	0,09	0,05	0,05	0,06				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,80	0,80	0,80	0,80	0,80	0,76	0,76	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,08	0,08	0,08	0,08	0,13	0,13	0,12				
Power	MWh																										1,18	0,12	0,29	0,78

Table 9-9 DMR; Fuelled with HFO; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	27	893	893	580	696	30	30	30	30	30	-30	-30	10	150	-30	25	670	943	893	677	361	361	580	696				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,41	1,24	1,24	1,24	2,79	6,36	6,36	1,91	4,44	0,83	3,62	3,02	0,60	0,15	1,40	0,45	0,18	35,51	35,51	35,51	35,51	35,51	38,45	38,45	34,89				
Molar Flow	kmol/h	25,68	48,20	48,20	82,57	167,72	227,30	227,30	106,19	121,11	22,53	98,58	69,12	29,47	7,37	77,78	22,10	10,97	1277,56	1273,42	1273,42	1273,42	1273,42	1333,86	1333,86	1244,49				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,38	0,38	0,00	0,38	1,00	0,02	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,01	0,03	0,03	0,03	0,03	0,05	0,05	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,27	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	0,00	0,00	0,00	0,46	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,06	0,09	0,09	0,09	0,09	0,05	0,05	0,06				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,80	0,80	0,80	0,80	0,80	0,76	0,76	0,82				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,08	0,08	0,08	0,08	0,13	0,13	0,12				
Power	MWh																										2,24	0,22	0,60	1,40

9.4 DMR with recycle – HFO

Table 9-10 DMR with recycle; Fuelled with HFO; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	708	30	30	30	30	30	-30	-30	10	150	10	25	25	15	943	586	361	396	580	708	508	361				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,17	0,51	0,51	0,51	1,15	2,61	2,61	0,79	1,82	0,34	1,48	1,24	0,25	0,06	0,58	0,19	0,05	1,65	1,88	1,88	1,88	11,83	13,71	13,71	12,25	12,25	12,25				
Molar Flow	kmol/h	10,52	19,74	19,74	33,83	69,03	93,47	93,47	43,91	49,56	9,22	40,34	28,31	12,03	3,01	32,20	9,02	3,12	57,05	69,18	70,39	70,39	410,22	480,61	480,61	443,95	443,96	443,96				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,39	0,39	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,01	0,04	0,04	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,10	0,10	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,26	0,26	0,00	0,26	0,00	0,00	0,03	0,04	0,04	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,47	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,18	0,18	0,05	0,07	0,07	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,0	0,00	0,00	0,00	0,0	0,00	0,0	0,0	0,79	0,65	0,64	0,64	0,76	0,75	0,75	0,81	0,81	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,0	0,00	0,00	0,00	0,0	0,00	0,0	0,0	0,21	0,17	0,00	0,00	0,13	0,11	0,11	0,09	0,09	0,09				
Power	MWh																												1,00	0,10	0,24	0,66

Table 9-11 DMR with recycle; Fuelled with HFO; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	707	30	30	30	30	30	-30	-30	10	150	10	25	25	15	943	601	361	400	580	707	511	361				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,35	1,04	1,04	1,04	2,36	5,37	5,37	1,63	3,74	0,70	3,04	2,54	0,51	0,13	1,20	0,38	0,13	3,48	3,98	3,98	3,98	24,37	28,35	28,35	25,35	25,35	25,35				
Molar Flow	kmol/h	21,60	40,55	40,55	69,47	141,98	192,16	192,16	90,38	101,79	18,94	82,85	58,14	24,71	6,18	66,33	18,53	7,79	120,61	146,94	151,46	151,46	845,21	996,67	996,67	921,39	921,40	921,40				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,38	0,38	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,01	0,05	0,05	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,10	0,10	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,26	0,26	0,00	0,26	0,00	0,00	0,03	0,06	0,06	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,47	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,07	0,07	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,63	0,63	0,76	0,74	0,74	0,80	0,80	0,80				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,17	0,00	0,00	0,13	0,11	0,11	0,09	0,09	0,09				
Power	MWh																												2,06	0,50	0,21	1,35

Table 9-12 DMR with recycle; Fuelled with HFO; 60% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	707	30	30	30	30	30	-30	-30	10	150	10	25	25	16	943	605	361	401	580	707	512	361				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,53	1,60	1,60	1,60	3,62	8,22	8,22	2,50	5,73	1,07	4,66	3,89	0,78	0,19	1,83	0,58	0,20	5,39	6,17	6,17	6,17	37,40	43,57	43,57	38,97	38,97	38,97				
Molar Flow	kmol/h	33,09	62,11	62,11	106,41	217,68	294,54	294,54	138,62	155,92	29,02	126,90	89,05	37,85	9,46	101,80	28,39	12,65	186,70	227,74	235,70	235,70	1297,15	1532,85	1532,85	1417,56	1417,56	1417,56				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,38	0,38	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,01	0,05	0,05	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,09	0,09	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,26	0,26	0,00	0,26	0,00	0,00	0,03	0,06	0,06	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,47	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,07	0,07	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,63	0,63	0,76	0,74	0,74	0,80	0,80	0,80				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,0	0,00	0,00	0,00	0,21	0,17	0,00	0,00	0,13	0,11	0,11	0,09	0,09	0,09				
Power	MWh																												3,15	0,32	0,77	2,07

Table 9-13 DMR with recycle; Fuelled with HFO; 80% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	707	30	30	30	30	30	-30	-30	10	150	10	25	25	16	943	609	361	402	580	707	513	361				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,72	2,17	2,17	2,17	4,93	11,18	11,18	3,39	7,78	1,45	6,33	5,28	1,05	0,26	2,49	0,79	0,29	7,39	8,46	8,46	8,46	50,80	59,26	59,26	53,01	53,01	53,01				
Molar Flow	kmol/h	44,98	84,42	84,42	144,63	295,79	400,26	400,26	188,34	211,92	39,44	172,48	121,04	51,45	12,86	138,29	38,59	17,77	255,98	312,33	323,81	323,81	1762,10	2085,91	2085,91	1929,20	1929,20	1929,20				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,38	0,38	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,01	0,05	0,05	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,09	0,09	0,05	0,06	0,06	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,26	0,26	0,00	0,26	0,00	0,00	0,03	0,06	0,06	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,47	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,17	0,17	0,05	0,07	0,07	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,62	0,62	0,76	0,74	0,74	0,80	0,80	0,80				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,17	0,00	0,00	0,13	0,11	0,11	0,09	0,09	0,09				
Power	MWh																												4,28	0,43	1,04	2,81

9.5 eSMR - HFO

Table 9-14 eSMR; Fuelled with HFO; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	675	453	30	30	30	-30	10	361	580	675	439	361					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,10	0,45	0,78	0,78	0,78	0,78	0,78	2,24	2,24	2,24	0,68	1,56	1,34	0,23	15,80	15,80	14,34	14,34	14,34					
Molar Flow	kmol/h	6,28	25,12	44,04	44,04	44,04	56,60	56,61	81,02	81,02	81,02	37,66	43,36	30,71	12,65	547,95	547,95	511,33	511,33	511,33					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,13	0,13	0,04	0,04	0,04	0,00	0,08	0,02	0,21	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,76	0,97	0,25	0,05	0,05	0,01	0,01	0,01					
H₂		0,00	0,00	0,16	0,16	0,16	0,48	0,48	0,09	0,09	0,09	0,00	0,16	0,00	0,55	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,30	0,30	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,05	0,05	0,06	0,06	0,06					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,76	0,76	0,82	0,82	0,82					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,13	0,13	0,12	0,12	0,12					
Power	MWh																				1,08	0,51	0,11	0,26	0,20

Table 9-15 eSMR; Fuelled with HFO; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	675	453	30	30	30	-30	10	361	580	675	439	361					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,20	0,92	1,57	1,57	1,57	1,57	1,57	4,53	4,53	4,53	1,37	3,16	2,70	0,45	31,98	31,98	29,03	29,03	29,03					
Molar Flow	kmol/h	12,71	50,85	89,04	89,04	89,04	114,46	114,46	163,89	163,89	163,89	76,23	87,66	62,18	25,48	1109,43	1109,43	1035,30	1035,30	1035,30					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,13	0,13	0,04	0,04	0,04	0,00	0,08	0,02	0,21	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,76	0,97	0,25	0,05	0,05	0,01	0,01	0,01					
H₂		0,00	0,00	0,16	0,16	0,16	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,54	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,30	0,30	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,05	0,05	0,06	0,06	0,06					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,76	0,76	0,82	0,82	0,82					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,13	0,13	0,12	0,12	0,12					
Power	MWh																				2,18	1,03	0,22	0,53	0,41

Table 9-16 eSMR; Fuelled with HFO; 60% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	675	454	30	30	30	-30	10	361	580	675	439	361					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,31	1,38	2,37	2,37	2,37	2,37	2,37	6,83	6,83	6,83	2,07	4,76	4,08	0,68	48,24	48,24	43,78	43,78	43,78					
Molar Flow	kmol/h	19,16	76,66	133,72	133,72	133,72	172,05	172,05	246,59	246,59	246,59	114,91	131,68	93,77	37,91	1673,32	1673,32	1561,52	1561,52	1561,52					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,13	0,13	0,04	0,04	0,04	0,00	0,07	0,02	0,20	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,76	0,97	0,25	0,05	0,05	0,01	0,01	0,01					
H₂		0,00	0,00	0,15	0,15	0,15	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,54	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,30	0,30	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,05	0,05	0,06	0,06	0,06					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,76	0,76	0,82	0,82	0,82					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,13	0,13	0,12	0,12	0,12					
Power	MWh																				3,29	1,55	0,33	0,80	0,61

Table 9-17 eSMR; Fuelled with HFO; 80% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	675	454	30	30	30	-30	10	361	580	675	439	361					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,41	1,85	3,17	3,17	3,17	3,17	3,17	9,14	9,14	9,14	2,77	6,37	5,46	0,91	64,58	64,58	58,61	58,61	58,61					
Molar Flow	kmol/h	25,65	102,60	179,12	179,12	179,12	230,42	230,42	330,18	330,18	330,18	153,81	176,37	125,50	50,87	2239,98	2239,98	2090,35	2090,35	2090,35					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,13	0,13	0,04	0,04	0,04	0,00	0,08	0,02	0,20	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,76	0,97	0,25	0,05	0,05	0,01	0,01	0,01					
H₂		0,00	0,00	0,15	0,15	0,15	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,54	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,30	0,30	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,05	0,05	0,06	0,06	0,06					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,76	0,76	0,82	0,82	0,82					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,13	0,13	0,12	0,12	0,12					
Power	MWh																				4,40	2,07	0,44	1,07	0,82

9.6 SMR – LNG

Table 9-18 SMR; Fuelled with LNG; 20% CO₂ capture target

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	E1	E2	E3	E4
T	C	25	144	114	800	800	580	663	30	30	30	-30	-30	-30	-30	25	649	850	803	581	360	360	580	663				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,07	0,31	0,38	0,38	0,38	0,48	1,39	1,39	0,44	0,94	0,81	0,14	0,10	0,03	0,07	10,47	10,47	10,47	10,47	10,47	11,28	11,28	10,37				
Molar Flow	kmol/h	4,29	17,16	21,45	21,45	30,02	36,10	51,29	51,29	24,63	26,65	18,56	8,09	6,07	2,02	4,15	378,97	378,19	378,19	378,19	378,19	395,58	395,58	372,80				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,23	0,23	0,23	0,00	0,01	0,02	0,02	0,02	0,02	0,04	0,04	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,51	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,07	0,10	0,10	0,10	0,10	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,80	0,80	0,80	0,80	0,80	0,77	0,77	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,08	0,08	0,08	0,08	0,12	0,12	0,11				
Power	MWh																								0,66	0,07	0,16	0,44

Table 9-19 SMR; Fuelled with LNG; 40% CO₂ capture target

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	E1	E2	E3	E4
T	C	25	144	114	800	800	580	663	30	30	30	-30	-30	-30	-30	25	648	850	804	582	360	360	580	663				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,14	0,63	0,77	0,77	0,77	0,98	2,83	2,83	0,91	1,93	1,65	0,28	0,21	0,07	0,14	21,73	21,73	21,73	21,73	21,73	23,37	23,37	21,52				
Molar Flow	kmol/h	8,76	35,06	43,82	43,82	61,33	73,62	104,69	104,69	50,35	54,35	37,96	16,38	12,29	4,10	8,70	786,40	784,84	784,84	784,85	784,85	820,20	820,20	773,61				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,01	0,02	0,02	0,02	0,02	0,04	0,04	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,51	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,07	0,10	0,10	0,10	0,10	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,80	0,80	0,80	0,80	0,80	0,77	0,77	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,08	0,08	0,08	0,08	0,12	0,12	0,11				
Power	MWh																								1,35	0,14	0,32	0,89

Table 9-20 SMR; Fuelled with LNG; 60% CO₂ capture target

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	E1	E2	E3	E4
T	C	25	144	114	800	800	580	661	30	30	30	-30	-30	-30	-30	25	647	850	805	584	360	360	580	661				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,21	0,96	1,17	1,17	1,17	1,48	4,30	4,30	1,38	2,92	2,51	0,42	0,31	0,10	0,22	34,03	34,03	34,03	34,03	34,03	36,53	36,53	33,71				
Molar Flow	kmol/h	13,30	53,20	66,50	66,50	93,07	111,50	158,71	158,71	76,46	82,25	57,68	24,58	18,43	6,14	13,59	1231,77	1229,44	1229,44	1229,28	1229,28	1282,86	1282,86	1212,03				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,01	0,02	0,02	0,02	0,02	0,04	0,04	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,51	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,07	0,10	0,10	0,10	0,10	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,80	0,80	0,80	0,80	0,80	0,77	0,77	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,08	0,08	0,08	0,08	0,12	0,12	0,11				
Power	MWh																								2,04	0,20	0,49	1,35

9.7 SMR with recycle – LNG

Table 9-21 SMR with recycle; Fuelled with LNG; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	668	30	30	30	-30	-30	-30	-30	25	25	21	850	302	360	355	580	668	427	360				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,06	0,27	0,33	0,33	0,33	0,42	1,20	1,20	0,39	0,82	0,70	0,12	0,09	0,03	0,03	0,73	0,79	0,79	0,79	8,26	9,04	9,04	8,26	8,26	8,26				
Molar Flow	kmol/h	3,72	14,89	18,61	18,61	26,04	31,31	44,46	44,46	21,38	23,08	16,07	7,02	5,26	1,75	1,86	25,14	28,75	28,08	28,08	289,82	317,90	317,90	298,16	298,16	298,16				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,23	0,23	0,23	0,00	0,00	0,01	0,09	0,09	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,51	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,03	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,77	0,76	0,76	0,81	0,81	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,12	0,11	0,11	0,10	0,10	0,10				
Power	MWh																										0,57	0,06	0,14	0,38

Table 9-22 SMR with recycle; Fuelled with LNG; 40% CO₂ capture target

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	669	30	30	30	-30	-30	-30	-30	25	25	21	850	270	360	352	580	669	424	360				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,12	0,54	0,66	0,66	0,66	0,84	2,42	2,42	0,78	1,64	1,41	0,24	0,18	0,06	0,06	1,38	1,50	1,50	1,50	16,63	18,13	18,13	16,55	16,55	16,55				
Molar Flow	kmol/h	7,49	29,97	37,46	37,46	52,43	63,04	89,53	89,53	43,04	46,49	32,35	14,14	10,61	3,54	3,52	47,95	55,01	53,65	53,65	583,40	637,06	637,06	597,32	597,33	597,33				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,23	0,23	0,23	0,00	0,00	0,01	0,09	0,09	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,51	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,77	0,76	0,76	0,81	0,81	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,12	0,11	0,11	0,10	0,10	0,10				
Power	MWh																										1,16	0,12	0,28	0,77

Table 9-23 SMR with recycle; Fuelled with LNG; 60% CO₂ capture target

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	668	30	30	30	-30	-30	-30	-30	25	25	21	850	277	360	353	580	668	424	360				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,18	0,82	1,00	1,00	1,00	1,27	3,66	3,66	1,17	2,48	2,13	0,36	0,27	0,09	0,09	2,11	2,29	2,29	2,29	25,48	27,77	27,77	25,38	25,38	25,38				
Molar Flow	kmol/h	11,32	45,29	56,61	56,61	79,23	95,17	135,23	135,23	65,06	70,17	48,91	21,27	15,95	5,32	5,39	73,25	83,95	81,93	81,93	894,55	976,48	976,48	916,39	916,38	916,38				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,23	0,23	0,23	0,00	0,00	0,01	0,09	0,09	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,51	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,04	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,77	0,76	0,76	0,81	0,81	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,12	0,11	0,11	0,10	0,10	0,10				
Power	MWh																										1,75	0,18	0,42	1,15

Table 9-24 SMR with recycle; Fuelled with LNG; 80% CO₂ capture target

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	144	114	800	800	580	666	30	30	30	-30	-30	-30	-30	25	25	21	850	291	360	354	580	666	425	360				
P	atm	1	4	1	1	1	1	1	1	1	1	25	25	25	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,24	1,10	1,34	1,34	1,34	1,70	4,91	4,91	1,58	3,34	2,86	0,48	0,36	0,12	0,12	2,91	3,14	3,14	3,14	35,27	38,41	38,41	35,20	35,20	35,20				
Molar Flow	kmol/h	15,20	60,80	76,00	76,00	106,36	127,56	181,45	181,45	87,43	94,02	65,75	28,27	21,20	7,07	7,47	100,68	115,22	112,53	112,53	1239,21	1351,73	1351,73	1270,91	1270,91	1270,91				
CH₄		1,00	0,00	0,20	0,20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,00	0,06	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,00	0,00	0,00	0,08	0,10	0,04	0,04	0,00	0,07	0,02	0,19	0,19	0,19	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,00	0,00	0,00	0,06	0,09	0,39	0,39	0,00	0,75	0,97	0,24	0,24	0,24	0,00	0,00	0,01	0,09	0,09	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,00	0,00	0,00	0,49	0,50	0,09	0,09	0,00	0,17	0,00	0,57	0,57	0,57	0,00	0,00	0,03	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	1,00	0,80	0,80	0,37	0,30	0,48	0,48	1,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,08	0,08	0,08				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,69	0,71	0,71	0,77	0,76	0,76	0,81	0,81	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,18	0,03	0,03	0,12	0,11	0,11	0,10	0,10	0,10				
Power	MWh																										2,34	0,23	0,56	1,54

9.8 DMR – LNG

Table 9-25 DMR; Fuelled with LNG; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	27	893	893	580	684	30	30	30	30	30	-30	-30	10	150	-30	25	661	943	901	686	361	360	580	684				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,14	0,41	0,41	0,41	0,92	2,10	2,10	0,63	1,46	0,27	1,19	0,99	0,20	0,05	0,46	0,15	0,08	13,71	13,71	13,71	13,71	13,71	14,66	14,66	13,48				
Molar Flow	kmol/h	8,46	15,87	15,87	27,20	55,38	75,04	75,04	35,19	39,85	7,41	32,44	22,76	9,68	2,42	25,76	7,26	4,73	496,73	495,38	495,38	495,38	495,38	514,24	514,24	484,74				
CH ₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,38	0,38	0,00	0,38	1,00	0,02	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,10	0,10	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO ₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,01	0,03	0,03	0,03	0,03	0,04	0,04	0,01				
H ₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,27	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H ₂ O		0,00	0,00	0,00	0,00	0,47	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,07	0,11	0,11	0,11	0,11	0,07	0,07	0,07				
N ₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,79	0,79	0,79	0,79	0,77	0,77	0,81				
O ₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,10	0,07	0,07	0,07	0,07	0,12	0,12	0,11					
Power	MWh																										0,79	0,08	0,20	0,51

Table 9-26 DMR; Fuelled with LNG; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	E1	E2	E3	E4
T	C	25	27	893	893	580	683	30	30	30	30	30	-30	-30	10	150	-30	25	660	943	902	688	360	360	580	683				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,28	0,84	0,84	0,84	1,90	4,32	4,32	1,31	3,01	0,56	2,45	2,05	0,40	0,10	0,96	0,30	0,16	28,73	28,73	28,73	28,73	28,73	30,69	30,69	28,27				
Molar Flow	kmol/h	17,37	32,54	32,54	55,79	114,21	154,70	154,70	72,92	81,79	15,17	66,62	46,86	19,75	4,94	53,48	14,82	10,09	1041,22	1038,49	1038,49	1038,49	1038,49	1077,06	1077,06	1016,32				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,39	0,39	0,00	0,39	1,00	0,02	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,10	0,10	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,01	0,03	0,03	0,03	0,03	0,04	0,04	0,01				
H₂		0,00	0,04	0,04	0,44	0,23	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,27	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	0,00	0,00	0,00	0,47	0,47	0,47	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,07	0,11	0,11	0,11	0,11	0,07	0,07	0,07				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,79	0,79	0,79	0,79	0,77	0,77	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,10	0,07	0,07	0,07	0,07	0,12	0,12	0,11				
Power	MWh																										1,62	0,16	0,41	1,05

9.9 DMR with recycle – LNG

Table 9-27 DMR with recycle; Fuelled with LNG; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	696	30	30	30	30	30	-30	-30	10	150	10	25	25	14	943	552	360	384	580	696	486	361				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,10	0,31	0,31	0,31	0,70	1,58	1,58	0,49	1,10	0,20	0,89	0,74	0,15	0,04	0,36	0,11	0,02	0,92	1,05	1,05	1,05	8,34	9,39	9,39	8,51	8,51	8,51				
Molar Flow	kmol/h	6,34	11,89	11,89	20,37	42,18	56,92	56,92	27,09	29,83	5,55	24,28	17,04	7,24	1,81	20,00	5,43	1,25	31,84	38,52	38,51	38,51	292,63	331,14	331,14	309,03	309,04	309,04				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,39	0,39	0,00	0,39	1,00	0,00	0,09	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,01	0,02	0,02	0,00	0,00	0,00	0,00	0,00	0,00				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,11	0,11	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,22	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,26	0,00	0,00	0,04	0,03	0,03	0,00	0,00	0,00	0,00	0,00	0,00				
H₂O		0,00	0,00	0,00	0,00	0,47	0,48	0,48	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,18	0,18	0,07	0,08	0,08	0,09	0,09	0,09				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,65	0,65	0,77	0,75	0,75	0,81	0,81	0,81				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,17	0,00	0,00	0,12	0,11	0,11	0,09	0,09	0,09				
Power	MWh																												0,56	0,06	0,15	0,39

Table 9-28 DMR with recycle; Fuelled with LNG; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	696	30	30	30	30	30	-30	-30	10	150	10	25	25	15	943	589	360	391	580	696	493	360				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,21	0,62	0,62	0,62	1,42	3,21	3,21	0,99	2,22	0,41	1,81	1,51	0,30	0,08	0,73	0,22	0,07	2,02	2,30	2,30	2,30	16,90	19,20	19,20	17,42	17,42	17,42				
Molar Flow	kmol/h	12,84	24,08	24,08	41,27	85,46	115,32	115,32	54,90	60,42	11,25	49,18	34,52	14,66	3,66	40,53	10,99	4,05	69,83	84,87	86,79	86,79	592,95	679,74	679,74	634,95	634,95	634,95				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,39	0,39	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,11	0,11	0,00	0,11	0,00	0,00	0,01	0,04	0,04	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,10	0,10	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,22	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,26	0,00	0,00	0,03	0,05	0,05	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,47	0,48	0,48	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,09	0,09	0,09				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,64	0,64	0,77	0,75	0,75	0,80	0,80	0,80				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,17	0,00	0,00	0,12	0,10	0,10	0,09	0,09	0,09				
Power	MWh																												1,20	0,12	0,30	0,79

Table 9-29 DMR with recycle; Fuelled with LNG; 60% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	694	30	30	30	30	30	-30	-30	10	150	10	25	25	16	943	605	360	394	580	694	495	360				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,31	0,94	0,94	0,94	2,17	4,88	4,88	1,51	3,37	0,63	2,74	2,29	0,45	0,11	1,12	0,34	0,11	3,20	3,65	3,65	3,65	26,02	29,67	29,67	26,96	26,96	26,96				
Molar Flow	kmol/h	19,50	36,58	36,58	62,69	130,44	175,79	175,79	83,99	91,80	17,08	74,71	52,43	22,28	5,57	62,19	16,71	7,11	110,85	134,66	138,47	138,47	913,50	1051,97	1051,97	983,95	983,95	983,95				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,39	0,39	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,10	0,10	0,00	0,11	0,00	0,00	0,01	0,04	0,04	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,10	0,10	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,22	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,26	0,00	0,00	0,03	0,06	0,06	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,48	0,48	0,48	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,09	0,09	0,09				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,63	0,63	0,77	0,75	0,75	0,80	0,80	0,80				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,21	0,17	0,00	0,00	0,12	0,10	0,10	0,09	0,09	0,09				
Power	MWh																												1,82	0,18	0,45	1,19

Table 9-30 DMR with recycle; Fuelled with LNG; 80% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	E1	E2	E3	E4
T	C	25	27	893	893	580	691	30	30	30	30	30	-30	-30	10	150	10	25	25	16	943	610	360	394	580	691	493	360				
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	25	1	25	1	1	1	1	1	1	1	1	1	1	1				
Mass Flow	t/h	0,42	1,26	1,26	1,26	2,91	6,53	6,53	2,03	4,51	0,84	3,67	3,06	0,61	0,15	1,50	0,45	0,16	4,32	4,94	4,94	4,94	36,16	41,10	41,10	37,47	37,47	37,47				
Molar Flow	kmol/h	26,10	48,96	48,96	83,91	174,72	235,43	235,43	112,55	122,87	22,87	100,01	70,18	29,83	7,46	83,36	22,37	9,99	149,76	182,12	187,87	187,87	1270,86	1458,73	1458,73	1367,67	1367,67	1367,67				
CH₄		1,00	0,59	0,59	0,13	0,08	0,06	0,06	0,00	0,11	0,11	0,11	0,00	0,39	0,39	0,00	0,39	1,00	0,00	0,10	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00				
CO		0,00	0,02	0,02	0,43	0,21	0,02	0,02	0,00	0,04	0,04	0,04	0,01	0,10	0,10	0,00	0,11	0,00	0,00	0,01	0,05	0,05	0,00	0,01	0,01	0,01	0,01	0,01				
CO₂		0,00	0,36	0,36	0,00	0,01	0,40	0,40	0,00	0,76	0,76	0,76	0,98	0,24	0,24	0,00	0,24	0,00	0,00	0,03	0,09	0,09	0,04	0,05	0,05	0,01	0,01	0,01				
H₂		0,00	0,04	0,04	0,44	0,22	0,04	0,04	0,00	0,08	0,08	0,08	0,00	0,27	0,27	0,00	0,26	0,00	0,00	0,03	0,06	0,06	0,00	0,01	0,01	0,01	0,01	0,01				
H₂O		0,00	0,00	0,00	0,00	0,48	0,48	0,48	1,00	0,00	0,00	0,00	0,01	0,00	0,00	1,00	0,00	0,00	0,00	0,00	0,17	0,17	0,07	0,08	0,08	0,09	0,09	0,09				
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,65	0,63	0,63	0,77	0,75	0,75	0,80	0,80	0,80				
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,0	0,00	0,00	0,0	0,21	0,17	0,00	0,00	0,12	0,10	0,10	0,09	0,09	0,09				
Power	MWh																												2,43	0,24	0,61	1,58

9.10 eSMR - LNG

Table 9-31 eSMR; Fuelled with LNG; 20% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	665	443	30	30	30	-30	10	361	580	665	431	361					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,06	0,25	0,42	0,42	0,42	0,42	0,42	1,22	1,22	1,22	0,37	0,85	0,73	0,12	10,16	10,16	9,36	9,36	9,36					
Molar Flow	kmol/h	3,45	13,79	24,00	24,00	24,00	30,89	30,89	44,29	44,29	44,29	20,74	23,56	16,80	6,76	356,69	356,69	336,57	336,57	336,57					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,12	0,12	0,04	0,04	0,04	0,00	0,07	0,02	0,20	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,77	0,97	0,25	0,04	0,04	0,01	0,01	0,01					
H₂		0,00	0,00	0,15	0,15	0,15	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,55	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,31	0,31	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,07	0,07	0,07	0,07	0,07					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,77	0,77	0,81	0,81	0,81					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,12	0,12	0,11	0,11	0,11					
Power	MWh																				0,58	0,28	0,06	0,14	0,10

Table 9-32 eSMR; Fuelled with LNG; 40% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	664	443	30	30	30	-30	10	360	580	664	430	360					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,11	0,47	0,81	0,81	0,81	0,81	0,81	2,33	2,33	2,33	0,71	1,62	1,39	0,23	19,46	19,46	17,94	17,94	17,94					
Molar Flow	kmol/h	6,55	26,20	45,60	45,60	45,60	58,70	58,69	84,20	84,20	84,20	39,42	44,78	31,94	12,85	683,09	683,09	644,82	644,82	644,82					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,12	0,12	0,04	0,04	0,04	0,00	0,07	0,02	0,20	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,77	0,97	0,25	0,04	0,04	0,01	0,01	0,01					
H₂		0,00	0,00	0,15	0,15	0,15	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,55	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,31	0,31	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,07	0,07	0,07	0,07	0,07					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,77	0,77	0,81	0,81	0,81					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,12	0,12	0,11	0,11	0,11					
Power	MWh																				1,10	0,53	0,11	0,27	0,19

Table 9-33 eSMR; Fuelled with LNG; 60% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	665	443	30	30	30	30	10	360	580	665	430	360					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	1	25	1	1	1	1	1					
Mass Flow	t/h	0,16	0,71	1,21	1,21	1,21	1,21	1,21	3,51	3,51	3,51	1,07	2,44	2,09	0,35	29,10	29,10	26,81	26,81	26,81					
Molar Flow	kmol/h	9,87	39,46	68,74	68,74	68,74	88,47	88,47	126,89	126,89	126,89	59,37	67,52	48,10	19,42	1021,58	1021,58	963,96	963,96	963,96					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,12	0,12	0,04	0,04	0,04	0,00	0,07	0,02	0,20	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,77	0,97	0,25	0,04	0,04	0,01	0,01	0,01					
H₂		0,00	0,00	0,16	0,16	0,16	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,55	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,57	0,57	0,57	0,30	0,30	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,07	0,07	0,07	0,07	0,07					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,77	0,77	0,81	0,81	0,81					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,12	0,12	0,11	0,11	0,11					
Power	MWh																				1,66	0,80	0,17	0,41	0,29

Table 9-34 eSMR; Fuelled with LNG; 80% CO₂ capture target.

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	E1	E2	E3	E4	E5
T	C	10	144	83	550	750	800	580	665	443	30	30	30	-30	10	360	580	665	430	360					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1					
Mass Flow	t/h	0,21	0,95	1,62	1,62	1,62	1,62	1,62	4,68	4,68	4,68	1,43	3,26	2,80	0,46	38,88	38,88	35,82	35,82	35,82					
Molar Flow	kmol/h	13,18	52,70	91,66	91,66	91,66	118,01	118,01	169,34	169,34	169,34	79,29	90,05	64,27	25,78	1364,52	1364,52	1287,53	1287,53	1287,53					
CH₄		1,00	0,00	0,14	0,14	0,14	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,06	0,12	0,12	0,04	0,04	0,04	0,00	0,07	0,02	0,20	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,77	0,97	0,25	0,04	0,04	0,01	0,01	0,01					
H₂		0,00	0,00	0,15	0,15	0,15	0,48	0,48	0,08	0,08	0,08	0,00	0,16	0,00	0,55	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,58	0,58	0,58	0,31	0,31	0,47	0,47	0,47	1,00	0,00	0,01	0,00	0,07	0,07	0,07	0,07	0,07					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,77	0,77	0,81	0,81	0,81					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,12	0,12	0,11	0,11	0,11					
Power	MWh																				2,22	1,07	0,22	0,55	0,38

9.11 Steel industry case study for on-land carbon capture

Table 9-35 Electrolysis system for carbon capture, steel industry case study

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	E1	E2	E3	E4	Electrolyser consumption
T	C	25	25	7	580	678	374	30	30	30	30	30	-30	10	25	25	10	430	295	580	678	366					
P	atm	1	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1	1	1	1					
Mass Flow	t/h	2,98	0,30	2,03	2,03	10,58	10,58	10,58	3,03	7,55	0,38	7,17	6,13	1,04	0,32	2,36	25,16	49,51	77,03	77,03	68,48	68,48					
Molar Flow	kmol/h	165,10	147,58	232,11	232,11	376,32	376,32	376,32	168,27	208,05	10,40	197,65	141,02	56,62	17,50	73,79	871,91	1785,70	2731,40	2731,40	2515,09	2515,09					
CH₄		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,06	0,06	0,04	0,04	0,04	0,00	0,08	0,08	0,08	0,02	0,22	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,10	0,10	0,42	0,42	0,42	0,00	0,77	0,77	0,77	0,97	0,25	0,00	0,00	0,00	0,09	0,06	0,06	0,01	0,01					
H₂		0,00	1,00	0,77	0,77	0,08	0,08	0,08	0,00	0,15	0,15	0,15	0,00	0,53	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
H₂O		1,00	0,00	0,08	0,08	0,45	0,45	0,45	1,00	0,00	0,00	0,00	0,01	0,00	1,00	0,00	0,00	0,18	0,12	0,12	0,13	0,13					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,79	0,72	0,72	0,72	0,78	0,78					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,00	0,21	0,01	0,10	0,10	0,08	0,08					
Power	MWh																						6,62	1,20	4,75	0,66	15,47

Table 9-36 eSMR , steel industry case study

	Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	E1	E2	E3	E4	E5
T	C	10	144	85	550	750	800	580	677	460	30	30	30	-30	10	430	10	251	580	677	323					
P	atm	1	4	1	1	1	1	1	1	1	1	1	1	25	25	1	1	1	1	1	1					
Mass Flow	t/h	0,58	2,61	4,40	4,40	4,40	4,40	4,40	12,84	12,84	12,84	3,95	8,89	7,68	1,20	49,51	42,57	92,09	92,09	83,65	83,65					
Molar Flow	kmol/h	36,28	145,12	244,23	244,23	244,23	316,79	316,79	458,57	458,57	458,57	219,27	239,30	176,47	62,83	1785,70	1475,64	3261,34	3261,34	3048,66	3048,66					
CH₄		1,00	0,00	0,15	0,15	0,15	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00					
CO		0,00	0,00	0,05	0,05	0,05	0,12	0,12	0,03	0,03	0,03	0,00	0,06	0,02	0,19	0,00	0,00	0,00	0,00	0,00	0,00					
CO₂		0,00	0,00	0,07	0,07	0,07	0,09	0,09	0,41	0,41	0,41	0,00	0,79	0,97	0,29	0,09	0,00	0,05	0,05	0,01	0,01					
H₂		0,00	0,00	0,13	0,13	0,13	0,48	0,48	0,07	0,07	0,07	0,00	0,14	0,00	0,52	0,00	0,00	0,00	0,00	0,00	0,00					
H₂O		0,00	1,00	0,59	0,59	0,59	0,31	0,31	0,48	0,48	0,48	1,00	0,00	0,01	0,00	0,18	0,00	0,10	0,10	0,10	0,10					
N₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,72	0,79	0,75	0,75	0,80	0,80					
O₂		0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01	0,21	0,10	0,10	0,08	0,08					
Power	MWh																					6,11	2,93	0,61	1,51	1,06