

**FEASIBILITY OF ADOPTING REFORMED
METHANOL-HIGH TEMPERATURE
PROTON EXCHANGE MEMBRANE FUEL
CELL TECHNOLOGY FOR THE PROPULSION
OF SEAGOING VESSEL**

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A dissertation submitted to the World Maritime University in partial fulfilment
of the requirements for the award of the degree of Master of Science in Maritime
Affairs

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Declaration

I certify that all the material in this dissertation that is not my own work has been identified, and that no material is included for which a degree has previously been conferred on me.

The contents of this dissertation reflect my own personal views, and are not necessarily endorsed by the University.

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Abstract

Title of Dissertation: **Feasibility of Adopting Reformed Methanol–High Temperature Proton Exchange Membrane Fuel Cells System for The Propulsion of Seagoing Vessel**

Degree: **Master of Science**

This study evaluates the technical, environmental and economic feasibility of an integrated methanol steam reformer and high-temperature proton exchange membrane fuel cells (HT-PEMFC) technology as an alternative to conventional marine engines. The mixed-methodology of this research employs process modelling of methanol steam reforming (MSR), simulating the electrochemical performance of HT-PEMFC, lifecycle assessment (LCA) and techno-economic assessment (TEA) under both market-driven and policy-driven scenarios. Expanding on past research, this study merges MSR and HT-PEMFC modelling with LCA and policy-sensitive TEA, evaluating the viability of sustainable (bio- and e-) methanol technologies.

This study found that onboard methanol reforming generated significant hydrogen output with tolerable carbon monoxide levels, that is suitable for downstream fuel-cell operation. The integrated system demonstrates superior efficiency compared with conventional marine engines, which suffer performance losses. On the environmental aspect, the lifecycle assessment reveals that green methanol pathways offer the highest mitigation potential, reducing well-to-wake (WtW) GHG emissions by 96–129% relative to baseline fuels, as bio-methanol achieved net-negative emissions depending on feedstock origin. Inversely, grey and blue methanol pathways performed similarly to baseline fuels, though being cheaper than green methanol in the absence of substantial carbon penalties.

The techno-economic analysis reveals that grey-methanol and conventional heavy fuel oil (HFO) propulsion technologies are the least costly in the baseline scenario, while sustainable methanol is constrained by capital intensity and elevated fuel prices. However, the introduction of market-based mechanisms considerably shifts competitiveness, improving the economic viability of sustainable alternatives. These results remain bounded by the simulation assumptions of this study, and evolving policy frameworks such as the IMO Net-Zero Framework, prone to refinement.

Overall, this study concludes that the feasibility of the integrated system depends on concurrent advances of scaling sustainable methanol production, supportive regulatory frameworks and technological durability. This study contributes novel insights by synthesising technical, operational, environmental and economic dimensions of fuel cell propulsion technologies, thereby, offering actionable guidance for industry stakeholders, policymakers and future researchers.

KEYWORDS: Decarbonisation, Methanol, Sustainable, Fuel Cells, GHG Emissions, LifeCycle Analysis, Techno-Economic Assessment, Policy.

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List of Abbreviations

ABS – American Bureau of Shipping

AC – Alternating Current

BV – Bureau Veritas

CAPEX – Capital Expenditure

CCS – Carbon Capture and Storage

CO – Carbon Monoxide

CO₂ – Carbon (IV) Oxide

CPH – Combined Power and Heat

DAC – Direct Air Capture

DC – Direct Current

DCS – Data Collection System

DNV – Det Norske Veritas

EEDI – Energy Efficiency Design Index

EU MRV – European Union (Reg. 2014/757) Monitoring, Reporting and Verification

GHG – Greenhouse Gases

HFO – Heavy Fuel Oil

HT-PEMFC – High Temperature Proton Exchange Membrane Fuel Cell

ICE – Internal Combustion Engine

IMO – International Maritime Organisation

IPCC – Intergovernmental Panel on Climate Change

ISO – International Standards Organisation

KR – Korean Register

kg - Kilogram

kW – Kilowatt

LCA – Life Cycle Assessment

LCOE - Levelized Cost of Energy

LHV – Lower Heating Value

LT-PEMFC – Low Temperature Proton Exchange Membrane Fuel Cell

MAN – Maschinenfabrik Augsburg-Nurnberg Energy Solutions

MD – Methanol Decomposition
MGO – Marine Gas Oil
MJ – Mega Joules
MSR – Methanol Steam Reforming
MW – Megawatts
OCV – Open Circuit Voltage
OECD – Organisation for Economic Co-operation and Development
ORC – Organic Rankine Cycle
PBI – Polybenzimidazole
PEMFC – Proton Exchange [Polymer Electrolyte] Membrane Fuel Cell
PM – Particulate Matter
SO_x – Sulfur (IV) Oxide
TCO – Total Cost of Ownership
TtW – Tank-to-Wake
WtT – Well-to-Tank
WGS – Water Gas Shift
WtW – Well-to-Wake

CHAPTER 1

INTRODUCTION

1.0 Background

The maritime industry, accounting for 3% of global greenhouse gas emissions (approximately 1.057 billion tonCO₂ emissions) (IPCC, 2023), faces intense pressure to decarbonise due to overdependence on fossil fuels. This percentage is expected to surge without mitigation, amid increasing global trade. Consequently, the International Maritime Organisation adopted the revised GHG Strategy (2023), aiming for net-zero emissions by 2050 through innovative technologies and renewable energy sources. Concurrently, the International Transport Forum (2018) emphasised the opportunities and urgency for sustainable technological innovations for maritime decarbonisation.

Consequently, alternative fuels are attracting attention. However, their use presents technical and environmental challenges (Chiong et al., 2021), including storage and handling issues with respect to existing infrastructure, low energy density, cost inefficiency, poor ignition and efficiency (Popek, 2024; Ampah et al., 2021). The magnitude of their Global Warming Potential (GWP) evaluated via Life Cycle Assessment (LCA) studies noted considerable variations, dependent on fuel sources—fossil-based sources show high emissions while renewables have lower footprints—underscoring the importance of cleaner production pathways (Chalaris et al., 2021; Cucinotta et al., 2024).

Conventional marine propulsion systems suffer inefficient energy usage as approximately 40% [chemical] energy is converted to mechanical power due to thermal losses. However, Kunze et al. (2012) suggested improvements using alternative fuels, electrochemical conversion and energy storage technologies. van Biert et al. (2016) and Xing et al. (2021) in support, noted that fuel cells—electrochemical devices circumvent mechanical and Carnot efficiency—directly

converting chemical energy into electricity, and achieves higher energy efficiencies (50–60%) with marginal air emissions.

Studies by Sunden (2019) and Elfakas et al. (2023) described how the electrochemical reactions between the anode and the cathode of a fuel cell generate electron flow (electricity) that powers loads, while ions are transported across the electrolyte to the electrodes, maintains charge balance. Their advantages include scalable power outputs through cell stacking, higher energy density compared to other energy storage technologies, continuous energy output with reactant supply, quieter operation and minimal maintenance (Sunden, 2019; van Biert et al., 2016).

Mature fuel cell technologies use hydrogen as fuel, but are limited by high cost, low volumetric energy density, storage challenges (corrosion, space and leakage) (Chong et al, 2021; Foretich et al., 2021). However, Sanchez et al. (2024) contrasted that alternatives like ammonia, methane, and methanol require exhaust treatment to achieve near-zero GHG emissions. Among these, methanol stands out—despite its toxicity and low flashpoint—due to easier transportation, storage and handling at ambient temperature, minimal refuelling time, availability, and hydrogen-carrier role (Blanco et al., 2023; Sanchez et al., 2024). However, most commercial methanol are fossil-sourced, raising lifecycle emissions concerns similar to fossil fuels, but methanol produced from CO₂ capture, renewable electricity, and biomass provides cleaner alternatives (McKinlay et al., 2022; Blanco et al., 2023; Wang et al., 2022).

1.1 Problem Statement

The maritime sector is increasingly compelled to decarbonise, advancing to explore alternative fuels, energy efficiency measures and other propulsion technologies. Their adoption is enthusiastic, but long-term feasibility and sustainability remain uncertain. Among the alternatives, propulsion by methanol-powered fuel cells offers promising operational and environmental benefits, merging higher efficiency with logistical simplicity.

Currently, there is insufficient assessment of methanol integration with high-temperature fuel cells on operational performance, lifecycle emission and economic viability. These dimensions are addressed separately by existing studies instead of holistically, confining decision-making of the technology. This research addresses this deficit by fusing technical modelling, lifecycle assessment and economic analysis to provide a comprehensive evaluation of the fuel cell feasibility for long-range marine propulsion. It will also provide valuable evidence to support policy and investment decision-making, contributing to maritime decarbonisation pathways in academic literature.

1.2 Research Aim and Objectives

1.2.1 Aim

The primary aim of this research is to evaluate the feasibility of integrating onboard methanol steam reforming (MSR) to power fuel cells for the propulsion of long-range vessels, by assessing its operational practicability, economic viability and environmental impact compared with a conventional propulsion system.

1.2.2 Objectives

1. Evaluate performance characteristics (power output, efficiency and reliability) of the MSR–Fuel cell system.
2. Analyse capital and operating expenditures, lifecycle cost and long-term financial viability relative to conventional propulsion systems.
3. Compare lifecycle emissions of the fuel cell system with conventional fuels.
4. Explore the role of bio-methanol and e-methanol in enhancing sustainability.

1.3 Research Questions

1. How does the integrated system compare with conventional propulsion system in power output and energy efficiency?
2. What is the lifecycle carbon footprint of the fuel cell system relative to conventional fuels?
3. How can fuel cells' sustainability be enhanced through policy-supported bio-methanol and e-methanol adoption?

4. What is the lifecycle cost of the fuel cell system compared to conventional fuels?

1.4 Research Methodology

This study adopts a mixed-methods approach by integrating quantitative and qualitative techniques to provide a comprehensive understanding of the feasibility of using methanol fuel cells for maritime propulsion. Quantitative techniques—integrated system simulation, LifeCycle Assessment and techno-economic modelling—evaluate operational performance, and quantify emissions and costs respectively. Thematic analysis and literature reviews (qualitative methods), however, offer profound comprehension into the circumstantial and acceptability challenges. This integration aligns with the exploratory and evaluative nature of the research objectives. This data triangulation ensures a comprehensive and contextually nuanced understanding of the integrated system's feasibility for marine propulsion.

1.5 Research Ethics

Data used in this study will be obtained from peer-reviewed, publicly available literature and industry reports. Modelling assumptions and uncertainties will be appropriately acknowledged by the researcher to ensure transparency. Ethical responsibility also includes the reliability of data gathered and avoiding misinterpretation of data or results.

1.6 Research Assumptions

1. Technically, the operational performance and efficiency of methanol fuel cells will be better than those of conventional engines. Existing safety guidelines and technological advancements manage the associated risks for methanol handling.
2. Environmentally, bio-methanol and e-methanol have lower carbon footprints relative to conventional fuel.
3. Economically, bio-methanol and e-methanol will become progressively available and cost-effective over time.
4. The best approach for evaluating the operational, environmental and economic feasibility is a mixed-method.
5. The result of the study will provide actionable recommendations for prompt adoption.

1.7 Limitations

1. Methanol fuel cell propulsion technology is immature, with the possibility of insufficient operational data for long-term comparison. Data from a few specific case studies may not apply to conventional seagoing vessels.
2. Fluctuating methanol [bio- and e-] prices and technology immaturity may affect economic projections.
3. Simplification of model (ideal gas behaviour, steady-state assumptions) may affect operational accuracy.

CHAPTER 2

LITERATURE REVIEW

2.0 Introduction

This chapter reviews literature on methanol as a marine fuel, fuel cell technologies, and their integration for shipboard propulsion. The technical and environmental performance, regulatory frameworks and industry adoption trends will be examined to contextualise their feasibility for seagoing vessels. Synthesising insights across technical, policy, operational, and economic dimensions identify key knowledge gaps that underpin this study.

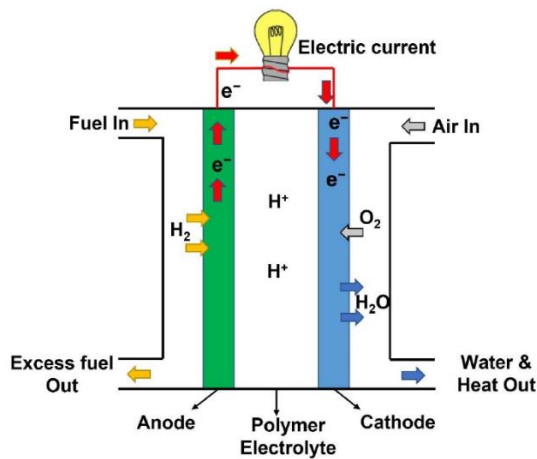
2.1 Fuel Cell Technology

According to Inal and Deniz (2020), fuel cells are classified based on their electrolyte types, working temperatures, fuel types or their area of application. However, commercially, electrolyte type is the basis for classification (de-Troya et al., 2016). The common types include Proton Exchange Membrane (PEMFC), Alkaline (AFC), Direct Methanol (DMFC), Phosphoric Acid (PAFC), Molten Carbonate (MCFC) and Solid Oxide (SOFC), reversible (functioning as fuel cells and electrolyser) and proton ceramic (Sunden, 2019; Inal & Deniz, 2022; Xing et al, 2021). However, Elfakas et al. (2023) noted that PEM Fuel Cells and Solid Oxide Fuel Cells (figures 1 and 2) are the extensively explored fuel cells for shipboard power systems. Each type has its distinct characteristics summarised in Appendix 1.

PEMFC typically operates at low temperatures (60–80°C), offering high power density, with dynamic response, suitable for shipboard propulsion (Benet et al., 2022; Inal & Deniz, 2022). Nevertheless, Xing et al. (2021) differentiated that the reliance on high-purity hydrogen, fuel purity vulnerability and CO poisoning presents substantial technical barriers for maritime applications, predominated by fuel flexibility and system robustness. Conversely, studies by Inal and Deniz (2022), and Perčić et al. (2022) highlighted SOFCs' fuel flexibility, higher efficiencies and internal reforming due to higher operating temperature (600–1000°C), but Elfakas et al. (2023)

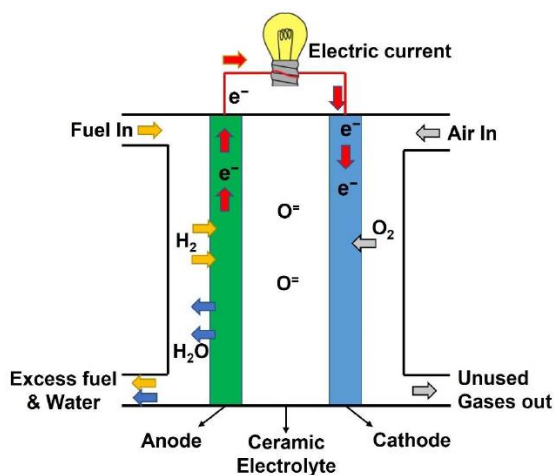
emphasised this result in thermal cycling, material degradation and longer start–up/shut–down period challenges. However, its suitability for long-range propulsion is strengthened by potential integration with combined heat and power (CPH) systems and gas turbine (Elfakas et al., 2023).

Figure 1: Basic Schematic diagram of PEMFC



Source: Elfakas et al. (2023)

Figure 2: Basic Schematic diagram of SOFC



Source: Elfakas et al. (2023)

Although LT-PEMFC offers dynamic efficiency, it suffers fuel purity constraints, while SOFC provides fuel versatility but challenged with material durability. HT-PEMFC operating at 110°C–200°C addresses the limitations of LT-PEMFC, allowing thermal integration with onboard methanol reformers. With thermal compatibility, they offer a thermodynamically synergistic configuration, reducing system complexity and enhancing efficiency. Additionally, van Biert et al. (2016) recognised HT-PEMFCs tolerate CO poisoning better than LT-PEMFCs, reducing fuel purification demands and enhancing maritime suitability.

2.2 Methanol as a Marine Fuel

2.2.1 Methanol Properties

Methanol (CH_3OH) has a boiling point of 65°C and is a simple, low-carbon and water-soluble alcohol, easing bunkering, transportation and storage at ambient temperature. Its sustainability for maritime applications is accentuated by rapid refuelling and widespread availability. It contains no nitrogen or sulfur, is a hydrogen carrier (Blanco et al., 2023; Sanchez et al., 2024), and aligns with safety and handling standards of conventional fuels (Popek, 2024). Deniz and Zincir (2016) further highlighted some favourable properties, including low viscosity, high stoichiometric fuel–air ratio, and high evaporative cooling. Despite these advantages, Foretich et al. (2021) and Ampah et al. (2021) recommended extensive safety measures—proper ventilation, reinforced fuel lines, and an advanced leak detection system—to mitigate its toxicity and flammability at room temperature. These studies reveal its carefully-managed technical feasibility for fuel cell applications with operational advantages and safety challenges. The comparative fuel properties in Appendix 2 buttress methanol's balance between energy density and safety.

2.2.2 Methanol Production Pathways

Classification of methanol is based on its production routes and associated carbon intensities, and is categorised into brown, grey, blue and green (bio- and e-) methanol as illustrated in Appendix 3.

2.2.2.1 Grey and Brown Methanol

Grey methanol is produced from fossil sources like natural gas, coke oven gas, LPG, and naphtha using steam reforming, autothermal reforming or partial oxidation, while brown methanol is produced via coal gasification. According to Methanol Institute (2022), steam reforming catalytically cracks natural gas with steam and CO₂ (upstream or downstream of the steam reformer, in the absence of oxygen) to produce synthesis gas. Autothermal reforming produces hydrogen-deficient synthesis gas, implying lower onboard reformer efficiency where high hydrogen yields are indispensable for fuel cell performance. Although commercially mature, these pathways are carbon-intensive and unsuitable for decarbonisation goals. Natural gas-sourced methanol emits approximately 103–110gCO₂/MJ (2000g–2200gCO₂eq/kg.methanol), while coal-based has three times larger carbon footprint at 300gCO₂/MJ, >5800gCO₂eq/kg.methanol (Methanol Institute, 2022).

2.2.2.2 Blue Methanol

Blue methanol is produced from green hydrogen (from renewable electricity via electrolysis) or blue hydrogen from Carbon Capture and Storage (CCS), with renewable or non-renewable CO₂. The International Energy Agency (2023) stated that integration with CCS can reduce lifecycle emissions up to 70%, dependent on storage integrity and capture efficiency.

2.2.2.3 Green (Bio- and E-) Methanol

Bio-methanol is produced from renewable sources such as biomass or municipal waste, gasified through renewable methanol synthesis. Similarly, e-methanol is produced from green hydrogen and Direct Air Capture (DAC), i.e., capturing of CO₂

from the air (Svanberg et al., 2018). Gasification of biomass for methanol synthesis achieves a 55–65% system efficiency, reducing carbon footprints significantly, relative to fossil-based routes (Khül et al., 2024).

2.2.3 Regulatory Policies and Industry Adoption

Novel regulatory frameworks like IMO's 2020 Interim Guideline for ships using methyl/ethyl alcohol as fuel (MSC.1/Circ.162) and the International Code for Ships using Gases or Other Low-Flashpoint Fuels widely support methanol adoption as marine fuel. Furthermore, classification societies advance their acceptance. DNV (Probst, 2022) added "Alternative Fuels for Containerships" class rules, and awarded an Approval-in-Principle (AiP) for PowerCell's methanol-to-power solution. Registro Italiano Navale (2022) approved the Freudenberg e-Power (methanol-powered fuel cell) System. These approvals represent a significant regulatory milestone but signal willingness for pilot projects rather than instantaneous large-scale deployment. Bureau Veritas (2024) issued design and operational classification rules (NR 670) for methanol/ethanol-fuelled vessels. Industry experts (Hyundai Heavy Industries, MAN Energy Solutions, Maersk Shipping Company, Wartsila, etc.) are progressively investing in methanol technologies.

2.3 Methanol Fuel Cell Integration in Maritime Applications

2.3.1 Electrical Supply and Propulsion Mechanism of Fuel Cell for Marine Vessels

Fuel cells convert chemical energy into electricity to power electrical propulsion motors and auxiliary onboard systems. The anodic hydrogen oxidation and cathodic oxygen reduction generate direct current (DC) electricity as electrons flow through an external circuit. Nonetheless, Tang et al. (2025) highlighted their performance is heavily dependent on operating conditions—temperature, pressure, hydrogen concentration and current density; whereas Zhang et al. (2025) demonstrated that series and parallel configurations of multiple fuel cell modules meet propulsion power requirements for medium-sized commercial vessels ranging to tens of megawatts.

Power electronics (DC/DC converters and inverters) condition the raw DC output from the fuel cell module to the required voltage and frequency of the propulsion system. The conditioned power drives synchronous or induction electric propulsion motors based on their torque–speed characteristics and integration compatibility with the fuel cell system (Jaurola et al., 2019). However, for onboard electrical usage (lighting, HVAC, and auxiliary machinery), the system converts DC power to AC power (Zhang et al., 2025). Technical guidelines for safe integration of fuel cell power systems–electrical isolation, ventilation and fault protection are provided by classification societies (ABS, 2023; BV, 2022; DNV, 2025; KR, 2022).

Marine propulsion load profiles are dynamic, influenced by sea/weather conditions, vessel’s speed and the operational profile, requiring a regulated fuel supply and dynamic current output. Dall'Armi et al. (2023) observed that modular fuel cell configuration enhances resilience even under partial failure, by enabling load sharing and redundancy. Moreover, integration with an energy management system (EMS) accelerates performance by harmonising thermal management, load demand, and power distribution. Truong et al. (2024) demonstrated that a multi-layered EMS structure significantly improves fuel efficiency and operational flexibility. underpinning the role of EMS integration in technical and economic optimisation.

2.3.2 Recent Methanol Fuel–Cell Technology Projects

- Blue World Technology: A 200-kW High-Temperature PEMFC system powered by green methanol was tested by this Danish company. Also, a 1MW system–its first pilot system of such magnitude–is scheduled to be installed on A.P. Moller–Maersk dual–fuel methanol vessels
- Freudenberg e–Power Systems: The approval from RINA marked a giant step towards commercial adoption of methanol–powered fuel cell systems in cruise ships and containerships (RINA, 2022).

- Sanlorenzo's Almax: Green methanol reformer fuel cell system is deployed on this 50-metre vessel, making it the first superyacht powered by methanol fuel cell.

2.3.3 Benefits and Limitations of Methanol Fuel Cell Technology

The adoption of methanol fuel cell technology offers operational and environmental advantages over conventional fuels and other gaseous alternative fuels. However, this transition is also associated with technical/operational and environmental complexities.

2.3.3.1 Benefits

Methanol-powered fuel cells offer significant benefits for shipboard applications, such as logistic simplicity and lower infrastructure cost compared to gaseous marine fuels (Methanol Institute, 2023). Furthermore, methanol's high energy density, lower flammability and water miscibility improve handling safety while enhancing considerable long-range voyage autonomy (Methanol Institute, 2023). Phogat et al. (2025) observed that these properties allow methanol to leverage existing supply chains and port infrastructure with minimal disruption. Environmentally, it emits lower levels of air emissions than MGO/HFO, with its biodegradable nature reducing risks in the event of accidental spills (Methanol Institute, 2023; Deniz & Zincir, 2016).

2.3.3.2 Technical Limitations

Methanol fuel cell applications face drawbacks despite their advantages. While its combustion in internal combustion engine (ICE) is cleaner than fossil fuels, its oxidation in a fuel cell also produces CO₂, limiting complete carbon neutrality unless integrated with offsetting strategies, e.g., biogenically-sourced (Phogat et al., 2025). They also highlighted that methanol fuel cells (particularly DMFCs) technically suffer lower power density and slower transit (dynamic) response, limiting their suitability for direct large-scale propulsion with better viability for hybrid (combination with batteries and ICEs) or auxiliary applications. Operationally, they are sensitive to load transients and thermal cycling. However, PEMFCs respond faster to variable loads

(Xu et al., 2023), with resultant reduced lifespan due to transient cycling and CO poisoning unless high-purity fuels are used.

Besides these limitations, DMFCs also face tenacious electrochemical and durability challenges, including membrane crossover (Phogat et al., 2025), where methanol molecules permeate the electrolyte membrane, undergoing parasitic oxidation (losses) at the cathode. This results in reduced efficiency and cell voltage, degradation of the electrolyte over time, and unproductive heat, wastes fuel and strains the system. Xing et al. (2021) also stressed that high-temperature methanol fuel cell technology (SOFCs) requires careful thermal management and specialised materials for durability under variable load cycles and harsh maritime environment (humidity, salinity and vibrations). Additionally, Phogat et al. (2025) stressed that methanol oxidation kinetics are less favourable to hydrogen, yielding greater overpotentials, lower cell voltages and overall system efficiency. A complex and costlier system is required to achieve equivalent performance to hydrogen fuel cells. Although hydrogen fuel cells outperform (minimal overpotential losses, higher cell voltage and efficiency, and zero-carbon emissions), infrastructural limitations, storage complexities and high-purity requirements restrain these advantages.

Consequently, Riel (2023) highlights that methanol fuel cells remedial include utilisation of methanol-tolerant catalyst (platinum-ruthenium alloy), advanced membranes with enhanced proton conductivity and reduced methanol permeability, and reformer-integrated systems, i.e., reformer-fuel cell to convert methanol into hydrogen-rich syngas, thus combining logistical advantages of methanol with superior performance of hydrogen fuel cells.

2.3.4 Challenges of Fuel Cells in Maritime Applications

Methanol fuel cell integration in the maritime context faces multidimensional challenges including scalability, economic and regulatory constraints. Methanol Institute (2023) noted that the economic barrier is paramount. Reliance on marine-

grade platinum-group catalyst and complex heat management units with an underdeveloped supply chain makes capital cost a stumbling block. (Benet et al., 2022; Wang et al., 2022). Perčić et al. (2022) resonating via LifeCycle Cost Assessment (LCCA) demonstrated the total cost of owning methanol-SOFC or DMFC vessel remains 27% –43% higher than diesel-powered ships. Although lifecycle costs are expected to decline with technological maturity and economies of scale, upfront investment may deter stakeholders in the absence of more robust policy incentives such as subsidies, carbon pricing mechanisms and green shipping corridors.

Secondly, regulatory standards are slow-paced. IMO, flag states and classification societies' guidelines for methanol onboard reformers, fuel ventilation, fire suppression and crew training are under development (Deniz & Zincir, 2016; Methanol Institute, 2023). The absence of universal benchmarks and uncertainties complicates project planning for shipowners.

van Biert et al. (2016) noted that methanol's volumetric energy density increases storage requirements in space-constrained ship designs. Perčić et al. (2022) and Xing et al. (2021) observed that improved tolerance to thermal cycling and fuel contaminants is a crucial concern for SOFCs and PEMFCs under variable loads and long-duration operations. However, Diesveld & De Maeyer (2020) highlighted that matching fuel cell technology with a vessel's operational profile is essential but increases complexity, emphasising the importance of policy-driven tools and detailed techno-economic assessments. Another challenge is inefficient water and heat management, particularly for DMFC. Haghighatjoo et al. (2025) reported that methanol crossover caused by membrane expansion and polarisation aggravates efficiency losses. However, addressing these challenges requires novelty in integration strategies, underscored by robust regulatory and policy frameworks

2.4 Methanol Fuel Cell versus Conventional Propulsion System – A Comparative Assessment

While section 2.3 examined the benefits and prevailing challenges of integrating methanol fuel cell within maritime application, this section contrasts this technology with conventional propulsion technologies, evaluating their relative efficiency, environmental performance, operational feasibility and economic viability. These aspects assess the future of methanol fuel cells in maritime decarbonisation strategies.

2.4.1 Energy Efficiency

Wang et al. (2024) observed that conventional marine diesel engines achieve thermal efficiency of 35%–45%, whereas fuel cells offer higher energy efficiency through circumventing the Carnot limit. High-temperature methanol fuel cells, such as SOFCs, achieve energy efficiencies exceeding 66% and exergy efficiency around 57% with optimised hybrid configuration (Qu et al., 2023; Wang et al., 2024). Similarly, an energy efficiency of 55.6%—under IMO Tier III NO_x compliance—was achieved by integrating a methanol fuel cell with a slow-speed two-stroke ICE engine, having a payback period of three years when carbon credits and incentives are considered (Qu et al., 2023). Integration with supercritical CO₂ Brayton cycles/ORC demonstrated an overall energy efficiency over 66% and power output capability above 65,000kW for an all-electric ship configuration, performance metrics not feasible with conventional marine diesel engines (Ma et al., 2024; and Phogat et al., 2025).

The thermodynamic benefits of hybridisation are underscored by these advantages, where waste heat from fuel cells enhances ICE intake air or drives auxiliary cycles. Remarkably, Ma et al. (2024) reported an EEDI of 5.94gCO₂/tonne.nm for high-temperature methanol fuel cell systems, reflecting alignment with the IMO's target. Fuel cells consistently outperform conventional diesel engines, as jointly suggested by these findings, although their commercial scaling is immature.

2.4.2 Environmental Profile and LifeCycle Assessment

Methanol-powered fuel cells proffer substantial lifecycle emission reductions relative to conventional marine fuels. A comparative LCA showed that bio-methanol lowers GHG emission reduction by approximately 85%, while e-methanol achieves 80–88.2% reduction when produced via renewable hydrogen and CO₂ capture (Strazza et al., 2010; Lee et al., 2024). Corbett and Winebrake (2018) also recognised that methanol use achieved 90–97% less SO_x and 90% less PM emissions with no methane slip, highlighting advantages over fossil-based propulsion systems.

Furthermore, hybrid configurations reduce tailpipe emissions, with net-zero carbon emissions in high-temperature fuel cells when powered by bio-methanol reformat (Araya et al., 2020). Its sustainability profile is further emphasised by compatibility with renewable sources (biomass gasification or DAC). Green methanol pathways reduce GHG by 80–88%, comparable to advanced biofuels as indicated by LCA consensus. These findings unequivocally support methanol's environmental superiority over conventional marine fuels, especially when green pathways are exploited.

2.4.3 Operational Feasibility

Despite initial technological complexity, methanol-powered fuel cells are garnering recognition for operational feasibility (fuel handling and logistics, safety, system integration, and performance). Its physical properties—described in section 2.2.1—make its bunkering and storage similar to conventional distillate fuels, necessitating only minimal infrastructural upgrades (Popek, 2024; Deniz & Zincir, 2016; Araya et al., 2020). This logistical simplicity contradicts ammonia or hydrogen, which require cryogenic or high-pressure storage. Its suitability for onboard reforming further enhances operational compatibility. Its steam reforming at low temperatures (200–300°C) yields approximately 70–80%vol of hydrogen with less catalyst degradation, enabling continuous fuel supply for high-temperature PEMFC systems, which tolerate impurities and provide steady power under variable loads (Ma et al., 2024).

Nonetheless, challenges—higher maintenance demands, thermal cycling, and slower transient response—persist compared to marine diesel ICEs. Modular hybridisation strategies—integrating energy storage or auxiliary ICEs—mitigate these issues, enhancing load-balancing and reliability (Diesveld & De Maeyer, 2020; Xing et al., 2021). Furthermore, recent developments by manufacturers (e.g., Ballard Power) suggest that the reformed-methanol and HT-PEMFC system achieves operational stability, lower maintenance, and long runtimes when paired with control and redundancy measures. This demonstrates their progressive readiness for propulsion and auxiliary shipboard power.

2.4.4 Economic Considerations

Due to the relative immaturity of fuel cell technologies and high costs of specialised components, the capital expenditure of methanol fuel cells remains considerably higher than conventional propulsion systems. However, integrating SOFC with ICEs showed payback periods of 2.2–3.1 years while accounting for fuel savings, carbon pricing, and incentives (Qu et al., 2023; Ma et al., 2024). Furthermore, Xing et al. (2021) ascertain that economic performance can be improved remarkably in short-sea and hybrid vessel applications with optimised storage facilities and power management strategies.

Additionally, operational economics are deterred by methanol cost. Historically, the price difference between methanol and HFO has been narrowing, due to stricter sulfur regulations ensuring lower prices relative to MGO and LNG despite volatility (Corbett & Winebrake, 2018). Flexible feedstock options (fossil-based sources, biomass/municipal waste, renewable electricity, CO₂ capture) and emerging green methanol markets promote supply chain resilience and long-term economic stability. Methanol supply chain optimisation modelling studies show domestically produced methanol with targeted subsidies achieves approximately 113% profitability improvement when compared with import-dominated supply chains (Villicani-Garcia et al., 2020).

Imminent competitiveness depends on incentive-based regulatory measures. Economic feasibility can be enhanced under emission trading schemes, as methanol's reduced carbon footprint translates directly to tangible financial benefit. Although the initial capital costs are exceptionally high, the long-term economic trajectory of high-temperature methanol fuel cells seem enthusiastic as regulatory frameworks increasingly promote fuel flexibility and carbon abatement. Fuel availability and emission pricing mechanisms will promote methanol fuel cell competitiveness, irrespective of high upfront costs.

2.5 Summary of Literature Review

The findings of this literature review align with the proposition of methanol as a practicable alternative fuel with substantial benefits over conventional fossil-based propulsion systems. The physicochemical characteristics of methanol provide distinguishable logistical advantages over gaseous alternative fuels, and its compatibility with existing bunkering and storage infrastructures reinforces the feasibility of its adoption without extensive overhauls.

Deployment of fuel cell technology instead of ICE ensures reduced thermal losses, greater energy and exergy efficiencies and near-silent operations. However, system complexities such as slower transient response, sensitivity to operational conditions and thermal management requirements offset these benefits. Lifecycle Analysis indicates significant reductions in air emissions (GHG and air pollutants), primarily when green methanol pathways are employed, aligning with global maritime decarbonisation goals. Nonetheless, high capital costs and a lack of standardised regulatory frameworks on emission pricing remain a critical bottleneck, delaying swift adoption and transitioning.

Although methanol-powered fuel cells offer a propitious pathway for sustainable maritime propulsion, their full-scale implementation for ocean-going vessels requires a holistic balance between lifecycle emission reductions, technical performance, and economic viability, which is limited in recent studies. This gap justifies the need for

holistic feasibility assessment of an integrated reformed-methanol HT-PEMFC system for maritime propulsion.

CHAPTER 3

METHODOLOGY

3.0 Research Design

Considering the multifaceted nature of this research, a mixed-methods approach is adopted, integrating thermodynamic/electrochemical modelling, lifecycle assessment, and techno-economic analysis. This ensures a comprehensive technical, environmental and economic evaluation. Thermodynamic modelling underpins the methodology to stimulate the performance of the reformed-methanol HT-PEMFC integrated system. This will provide insights into hydrogen yield, energy conversion efficiency, and scaling its output to meet the propulsion demands of a Panamax-sized vessel, directly informing research objective 1.

Comparative ISO 14040/44 LCA standards, augmented by IMO Guidelines on LifeCycle GHG Intensity of Marine Fuels (2024), address the environmental aspect. This compares the well-to-wake GHG emissions of the HT-PEMFC system to conventional propulsion systems, addressing research objectives 2 and 3. A techno-economic assessment (TEA) focusing on capital and operating expenditures, fuel costs, and payback periods (under policy scenarios-carbon levy) is performed to evaluate the economic viability, providing evidence for research objective 4.

This methodological triangulation ensures robustness-technical modelling identifying performance limits, LCA quantifying emissions, and TEA evaluating long-term viability. Together, this design provides a holistic feasibility assessment not attainable with a single approach. It builds directly on simulation results and comparative assessments presented in chapters 4 and 5.

3.1 Framework Overview

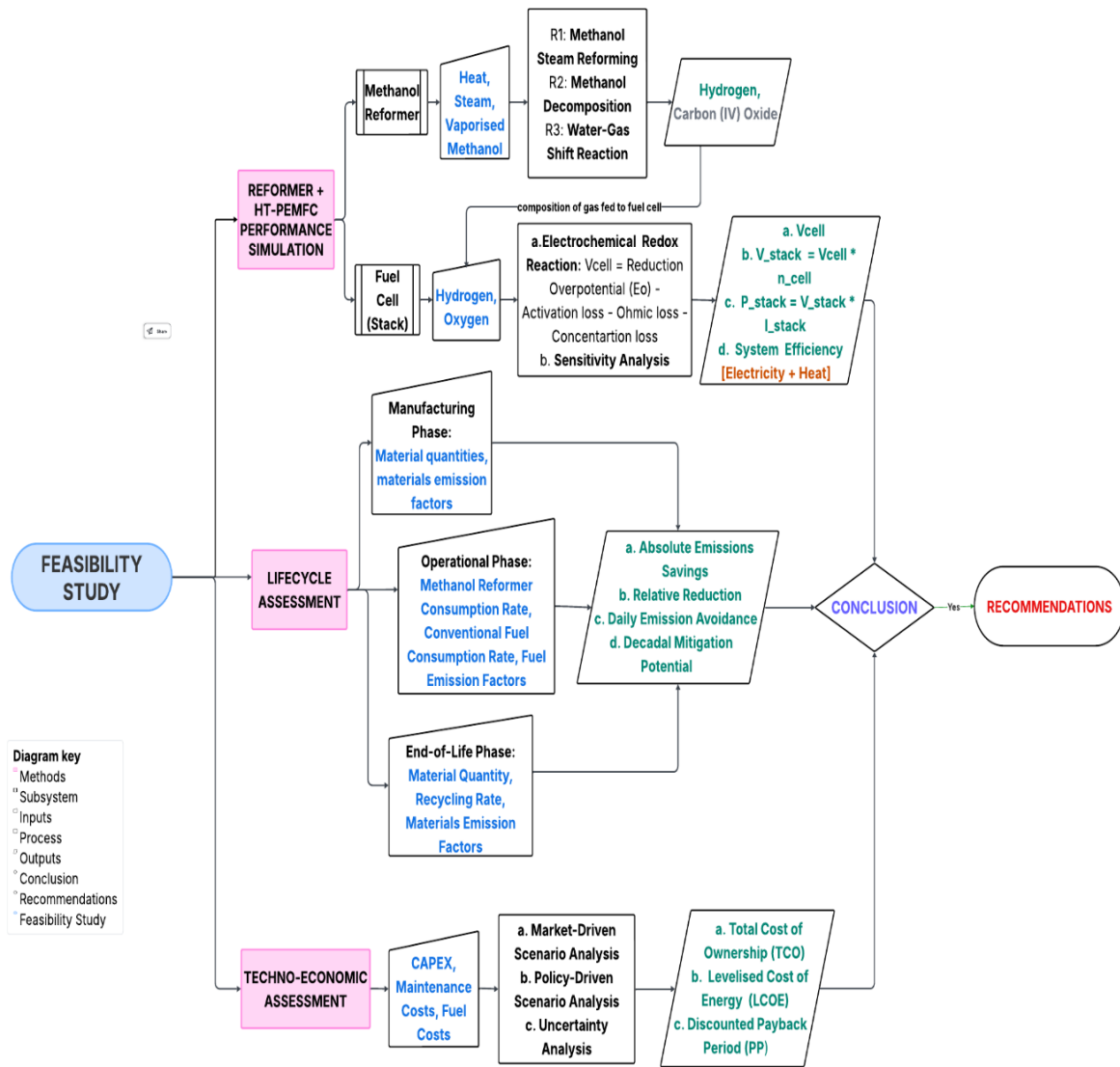
This research framework (Figure 4) adopts a model-based structure on four [core] methodological pillars: reformed-methanol and HT-PEMFC (stack) modelling, propulsion scaling, comparative emission analysis and economic/financial assessment.

1. Reformed-Methanol and HT-PEMFC Simulation: This involved modelling of steam methanol reforming for hydrogen production to power a fuel cell module under steady-state, and further simulates its performance. This will be implemented in Python programming language (Appendix 8-10) using libraries such as NumPy, SciPy, and Matplotlib for mathematical computation and visualisation.

2. Comparative Emission Analysis: This is comparing the lifecycle emission of methanol pathways (grey, blue bio-methanol and e-methanol) and the HT-PEMFC system to the well-to-wake of HFO/MGO.

3. Techno-Economic Assessment: Cost comparison is conducted using Python programming language (Appendices 8-9), to compare the total cost of ownership of the fuel cell system with conventional marine propulsion system.

Figure 3: Flowchart of the Methodological Framework



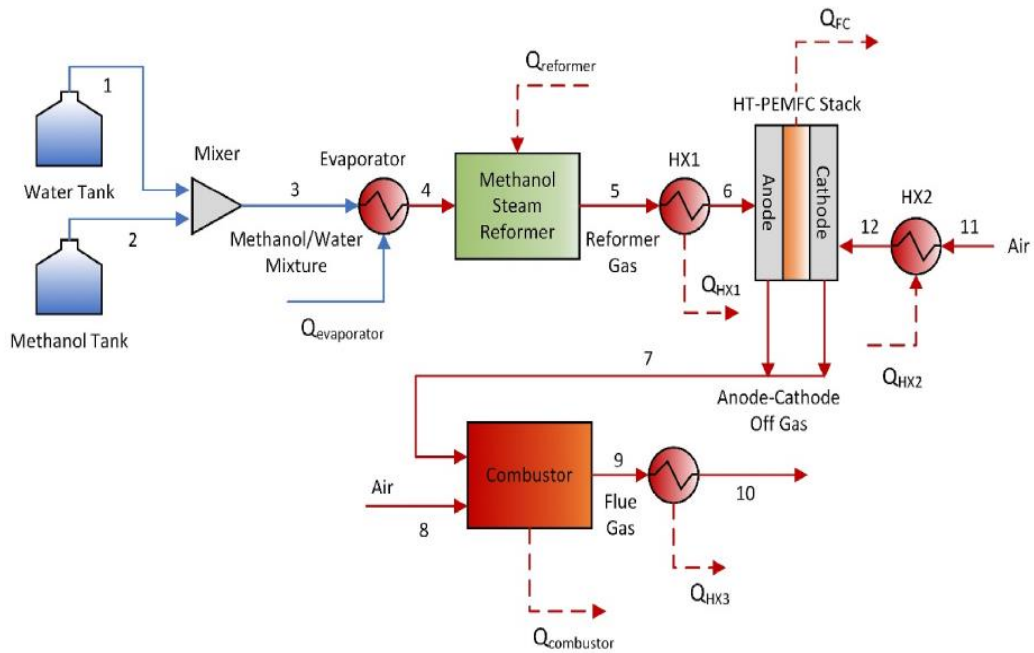
Source: Author

3.2 Reformed Methanol and HT-PEMFC System: Mathematical Modelling

The integrated system (Figure 3) comprises the methanol steam reformer, HT-PEMFC Stack, and their respective auxiliary systems. Although the core modelling of this study focuses on the methanol reformer and HT-PEMFC stack, the auxiliary systems

are significant in ensuring operational stability, safety and efficiency. These include the thermal management system (combustor, heat exchangers – evaporators, and coolant loops to recover waste heat and support onboard heating demands), air supply and humidification, pumps, fuel delivery system (manages pressurisation and maintains membrane hydration), and power conditioning units (DC/DC converters, inverters) (Jaurola et al., 2019; ABS, 2023; BV, 2022). The combustor provides adequate heat to kickstart the working of the reformer and maintain its working temperature (Zucconi et al., 2024), while the evaporator converts the aqueous methanol–water mixture into a homogenous gas (methanol_(vapour) and steam).

Figure 4: Schematic Diagram of the Integrated System

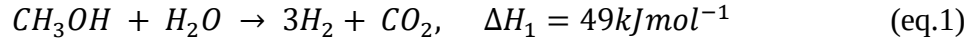


Sources: Li et al. (2023)

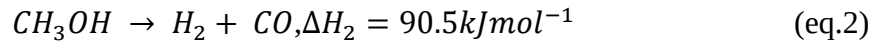
3.2.1 Methanol Reformer (MSR) Subsystem

The MSR subsystem is modelled as a one-dimensional plug flow reactor (PFR) that breaks methanol into hydrogen (reformat gas/fuel), CO and CO₂ using water and heat. It incorporated three key reactions – methanol steam reforming (eq.1), methanol decomposition (eq.2) and water–gas shift (eq.3).

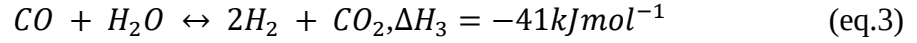
- Steam Reforming: This is an endothermic catalytic reaction characterised by low reaction temperature, high H₂ and low CO products. MSR is cheaper and produces more hydrogen mole per mole of methanol compared to other methanol-to-hydrogen production approaches (partial oxidation, and sorption-enhanced steam reforming). It is denoted by the equation below:



- Methanol Decomposition (an endothermic reaction)



- Water–Gas Shift (an exothermic reaction)



These reaction equations follow Arrhenius-based kinetics:

$$k_i = k_{i,0} \exp \left(- \frac{E_{a,i}}{RT} \right) \quad (eq.4)$$

where $k_{i,0}$ = Pre-exponential factor

$E_{a,i}$ = Activation energy

R = Ideal gas constant

T = temperature

The reaction rates (r_i) are denoted as $r_1 = k_1 C_{CH_3OH} C_{H_2O}$, $r_2 = k_2 C_{CH_3OH}$, and $r_3 = k_3 C_{CO} C_{H_2O}$ for the key reactions respectively.

The mass balance of the reactant and product species of the model along the reactor length (z) is denoted as equations 5-9:

$$\text{methanol: } \frac{dC_{CH_3OH}}{dz} = \frac{-r_1 - r_2}{u} \quad (eq.5)$$

$$\text{water vapour/steam: } \frac{dC_{H_2O}}{dz} = \frac{-r_1 - r_3}{u} \quad (eq.6)$$

$$\text{carbon monoxide: } \frac{dC_{CO}}{dz} = \frac{r_2 - r_3}{u} \quad (\text{eq.7})$$

$$\text{carbon (iv) oxide: } \frac{dCO_2}{dz} = \frac{r_1 + r_3}{u} \quad (\text{eq.8})$$

$$\text{hydrogen: } \frac{dC_{H_2}}{dz} = \frac{3r_1 + 2r_2 + r_3 - (A_m \cdot J_{H_2})}{u} \quad (\text{eq.9})$$

where u = superficial velocity, A_m = membrane area per unit length, J_{H_2} = hydrogen permeation flux, and $\frac{A_m \cdot J_{H_2}}{u}$ is the cumulative hydrogen permeation.

The hydrogen permeation flux (eq. 10) is related to the square root of the hydrogen partial pressure between the retentate and permeate sides [Sievert's law], and evaluated thus:

$$J_{H_2} = P_{H_2,perm} \left(\sqrt{p_{H_2,ret}} - \sqrt{p_{H_2,perm}} \right) \quad (\text{eq.10})$$

where $P_{H_2,perm}$ = hydrogen permeability constant, $p_{H_2,ret}$ = partial pressure of hydrogen on the retentate side, and $p_{H_2,perm}$ = hydrogen pressure on the permeate side.

Furthermore, a non-isothermal formulation captures the influence of the reaction heat and heat loss, and the energy balance (eq.11) is evaluated thus:

$$\frac{dT}{dz} = - \frac{Q_{rxn} + Q_{loss}}{u \cdot C_{p,total}} \quad (\text{eq.11})$$

However, $Q_{rxn} = r_1 \Delta H_1 + r_2 \Delta H_2 + r_3 \Delta H_3$, $Q_{loss} = U_{loss} (T_i - T_{ref})$ and

$$C_{p,total} = \alpha C_{p,gas} \sum_i C_i + (1 - \alpha) \rho_{cat} C_{p,cat},$$

where U_{loss} = overall heat loss coefficient, $C_{p,gas}$ = specific heat capacity of the gas phase (CH₃OH, H₂O, CO, CO₂, H₂), $C_{p,cat}$ = specific heat capacity of the catalyst bed, ρ_{cat} = catalyst bulk density and α = weighting factor between $C_{p,gas}$ and $C_{p,cat}$.

The modelling parameters and constants are obtained from literature (Li et al, 2023; Zhuang et al., 2023; Zhu et al., 2019). Some input parameters defined are temperature_{inlet} = 523.15K (250°C), pressure = 1atm, feed composition–CH₃OH =

2500mol/m³, H₂O = 3750mol/m³, steam-to-carbon ratio = 1.5, reactor length = 2.0m, diameter = 0.1m, while the complete parameters are tabulated in Appendix 4. The leading ordinary differential equations (ODEs)–mass and energy balance–describe the spatial evolution of species concentrations and temperature along the reactor length, and are solved using the function *solve_ivp*.

The performance metrics include methanol conversion rate (%), hydrogen yield, CO concentration (assessing compatibility with HT-PEMFC tolerance limits), temperature profile (identifying optimal heating zones and quasi-isothermal regions), and S/C ratio evolution (monitoring WGS enhancement and CO suppression). Afterwards, the partial pressure of hydrogen, i.e., the amount of hydrogen available to feed the fuel cell, is computed. Finally, sensitivity analyses are performed on S/C ratio (0.5–4.0) and inlet temperature (493–553K) to assess the impact on reformer performance.

3.2.2 HT-PEMFC Subsystem

This subsystem provides electricity for propulsion, low-temperature heat and by-product (water) from the electrochemical anodic hydrogen oxidation (eq.12) and cathodic oxygen reduction (eq.13). Electrochemical equations, Nernst and Butler–Volmer, were applied relating the fuel cell stack voltage and power to current density, accounting for activation, concentration and ohmic losses. Parameters like number of cells in a stack, active area of cell, oxygen pressure, Tafel slope, open circuit voltage, exchange current density and ohmic resistance were obtained from literature (Sunden, 2019; Cifuentes et al., 2023; Zhuang et al., 2023; Chen et al., 2024; Zhou et al., 2022). The efficiency of the subsystem is also simulated. The reactions at the anode and cathode of each fuel cell are described below:



The voltage (energy per unit charge) i.e., E_{nernst} was calculated by equation below:

$$E_{nernst} = E^o - \left(\frac{R \times T}{n \times F} \right) \times np.log(Q) \quad (eq.14)$$

where: E_{nernst} = reduction potential

E^o = standard cell potential

R = Ideal gas constant

T = temperature

n = ion charge (moles of electrons transferred in balanced redox)

F = Faraday's constant

Q = reaction quotient (measure of relative amounts of products and reactants

present in a reaction at a given time $\frac{PH_2 + (PO_2)^{0.5}}{PH_2O}$.

However, this voltage (eq.14) is affected by losses (Lotric, 2012). These include $\eta_{activation}$ —energy needed to start the reaction (calculated using Butler-Volmer equation) (eq.15), η_{ohmic} —resistance inside the cell due to ion migration across the electrolyte (eq.16) and $\eta_{concentration}$ —gas flow limitations, i.e., depletion of reactants due to mass transport (eq.17), which decreases the overall cell voltage (eq.18).

$$\eta_{act} = solve_eta_act(j, T_fc, j0, alpha_a, alpha_c) \quad (eq.15)$$

$$\eta_{ohmic} = j \times R_{ohmic} \quad (eq.16)$$

$$\eta_{conc} = \frac{R * T_fc}{n * F} \times np.log\left(\frac{1-j}{j_lim}\right) \quad (eq.17)$$

where j = current density, $j0$ = exchange current density $alpha_a$ = anode

charge transfer coefficient $alpha_c$ = cathode charge transfer coefficient

R_{ohmic} = area-specific resistance, j_lim = limiting current density.

The overall cell voltage is hence calculated:

$$V_{cell} = E_{nernst} - \eta_{act} - \eta_{ohmic} - \eta_{conc} \quad (eq.18)$$

The power produced by the stack (eq.19) was computed using a semi-empirical formulation with the stack voltage (eq.20) and current (eq.21).

$$V_{stack} = V_{cell} \times n_{cell} \quad (eq.19)$$

$$I_{total} = I_{stack} = j \times A_{cell} \quad (eq.20)$$

$$P_{total} = \frac{I_{total} \times V_{stack}}{1000} \text{ [kW]} \quad (\text{eq.21})$$

where V_{cell} is single cell voltage penalised by overpotentials, n_{cell} is the number of cells in a stack, j the current density, A_{cell} the active area per cell.

A loop was created to calculate voltage drops, power production, and hydrogen consumption for a range of current densities, and calculate the fuel efficiency at each current level. However, the hydrogen flow is constrained by Faraday's law governing the allowable current, described by the equation below:

$$I_{max} = ne \cdot F \cdot nH_2 \quad (\text{eq.22})$$

where F is Faraday's constant and ne is the number of electrons [i.e., 2 electrons per H_2 molecule].

The efficiency of the stack (eq.25) was calculated using the molar flow rate of hydrogen (eq.23) and the hydrogen energy used (eq.24) based on the Lower Heating Value (LHV) of hydrogen with the formulae below:

$$H_2 \text{ molar flow rate} = \frac{I_{total} \times n_{cell}}{2F} \quad (\text{eq.23})$$

$$PH_2 = \frac{H_2 \text{ mol rate} \times LHV_{H_2}}{1000} \text{ [kW]} \quad (\text{eq.24})$$

$$\text{Stack efficiency} = \frac{P_{total}}{PH_2}, \text{ if } PH_2 > 0 \text{ else } 0, \quad (\text{eq.25})$$

where

P_{total} is electrical power output and PH_2 is the energy value of the hydrogen used

3.2.3 Powertrain Scaling for a Panamax–Sized Vessel

The feasibility of the HT–PEMFC system for marine propulsion is assessed by linearly scaling the module–level output (~160kW) to match the propulsion demands (6MW) of a Panamax–class vessel, requiring 38modules in parallel configurations.

Under steady–state, HT–PEMFC stacks typically operate at 55–60% electrical efficiency (Zucconi et al., 2024). The required hydrogen energy input (eq.26) for a 6MW output is estimated using the LHV of hydrogen

$$\text{Hydrogen Energy Input} = \frac{P_{\text{output}} \times \text{hydrogen consumption rate}}{\gamma_{FC} \times \text{LHV } H_2} (\text{kWh}) \quad (\text{eq.26})$$

Since hydrogen is produced onboard, the daily methanol consumption is calculated based on the stoichiometry of the reforming reaction and the LHV of methanol (19.9MJ/kg).

3.2.4 Model Validation

To ensure the applicability and credibility of the developed fuel cell model, its outputs were comparatively benchmarked against the commercial PowerCell Group S3 system (2025a). The configuration of the datasheet (455 cells) corresponds with the cell count used in the simulation. This model replicated the key performance metrics of the 455-cell stack. The simulated power outputs ranged from 129–162kW, largely consistent with the rated and peak values (129–159kW) of the referenced system. The model's polarisation curve is comparable to the referenced voltage-current characteristics, with realistic cell voltage (~0.72V) and current density inputs. The model's fidelity is bolstered by temperature profiles and efficiency, which are within the specified bounds of the manufacturer. These demonstrate that the model represents real-world fuel cell behaviour, although theoretically robust. Referencing a commercial benchmark augments the validity and credibility of subsequent performance and optimisation analyses.

3.3 Comparative Lifecycle Analysis

3.3.1 Scope

This analysis assesses the mitigation potential of transitioning from fossil-based to electrochemical propulsion technologies, by quantifying HT-PEMFC's GHG emission reduction potentials to conventional HFO/MGO-fuelled systems.

3.3.2 Methodology

The analysis adopts an ISO 14040/44 standardised Lifecycle Assessment Framework, with a functional unit of 1 tonne-mile (transporting 1 tonne of cargo/nautical mile) to enable direct comparison between propulsion systems, while climate change impact

was quantified per kilogram of material and per tonne of fuel used. The framework boundaries include upstream fuel production and logistics (WtT), onboard conversion, lifecycle GHG emission of HT–PEMFC components and HFO/MGO fuels. Emission factors are sourced from Lifecycle Inventory Database and industry reports.

The analysis is categorised into manufacturing, operational, and end-of-life phases. The manufacturing and end-of-life phases calculate the emission of materials for the HT–PEMFC system, while operational discusses upstream and downstream fuels emissions. The upstream daily emission is calculated by multiplying the fuel quantity required for net output power by the average emission factor. The yearly emission is obtained by multiplying the daily emission by operational 250 sailing days, while the lifetime emission multiplies the consequent result by 25 years. The downstream yearly emission from combustion of conventional fuels is calculated by multiplying the emission factor by the daily consumption and the number of operational sailing days. The lifetime emission is calculated similarly to the upstream.

3.4 Techno-Economic Assessment

3.4.1 Scope

Financial comparison of reformed-methanol HT–PEMFC propulsion system and a conventional HFO/MGO marine engine will be conducted to complement this feasibility analysis by integrating deterministic and probabilistic modelling approaches. This aspect will evaluate capital expenditure (Methanol reformer, HT–PEMFC Modules and conventional marine engines), fuel costs, maintenance expenses, and the influence of carbon levy and subsidy structures over the expected vessel lifetime.

3.4.2 Methodology

The costs will be measured using the following metrics: Total Cost of Ownership (TCO), Levelized Cost of Energy (LCOE), and payback period. Data for this analysis

will be obtained from industry data and peer-reviewed literature. The LCOE is computed as $\frac{\text{total lifetime cost}}{\text{total lifetime energy output}}$ (\$/kWh).

3.4.2.1 Sensitivity Analysis

Monte Carlo simulation including fuel price variation ($\pm 10\%$), CAPEX Uncertainty ($\pm 10\%$), Fuel cell efficiency variation ($\pm 5\%$), will be simulated using Python programming language to assess the robustness of economic viability. TCO and LCOE period will be recalculated in each scenario to ascertain threshold contexts under which the HT-PEMFC system is considered superior. Cost comparison bar charts, payback period across fuel scenarios, and LCOE versus fuel price sensitivity curves will be visualised.

3.5 Methodology Assumptions and Limitations

The use of literature and open-access software applications, such as Python, led to the adoption of assumptions to simplify methodological complexity. These also incurred some limitations necessary to define the boundary of this study.

3.5.1 Key Assumptions

- I. Methanol Reformer – HT-PEMFC System: For a simplified analysis and computational tractability, the following assumptions were made:
 1. The model accounted for the operations of the reformer and HT-PEMFC stack/module, without considering auxiliary system demands to simplify the analysis.
 2. Steady-state conditions (no considerations of the significant transient effects of start-up and shut-down dynamics) were assumed, simplifying the modelling of reaction kinetics and the electrochemical performance. The operating conditions (temperature and pressure) of the HT-PEMFC stacks were assumed to be constant, with no significant variations in gas composition.
 3. Non-ideal interactions at high pressures were neglected, and the thermodynamic calculations simplified as all gaseous species in the reformer (CH_3OH , H_2O , CO , CO_2) were assumed to follow ideal gas behaviour.

4. Degradation of the catalyst (Cu/Zn/AlO₃) over time is not accounted for, as the catalyst in the MSR reactor was assumed to have uniform activity, ensuring consistent reaction rates throughout the reactor length.
5. Values for electrochemical parameters (Tafel slope, exchange current density, ohmic resistance, active area of cell, number of cells, etc.), and reaction kinetics were obtained from the literature.
6. CO and CO₂ (by-products) are assumed to be effectively managed respectively by PROX and sequestration, with minimal impact on the HT-PEMFC performance.
7. Potential inefficiencies at a larger scale are neglected as linear performance extrapolation from module-level (160kW) to vessel-level is assumed for the modular scaling of the HT-PEMFC stacks to meet the 6MW propulsion demand.

II. Comparative Lifecycle Analysis

1. Vessel construction, disposal and auxiliary power systems are not accounted for in this analysis, as the system boundary is defined as GHG well-to-wake (WtW) of fuels and the integrated MSR-Fuel cells system. Similarly, lifecycle emissions of BOP components/machinery of propulsion systems are excluded from this analysis.
2. Fuel pathways emission factors are assumed constant, based on midpoint industry estimates, neglecting regional variation.

III. Techno-Economic Modelling

1. Economies or diseconomies of scale are not accounted for as capital cost of each HT-PEMFC module is assumed constant based on current manufacturer projections.
2. Redundancy and overheads are neglected as yearly maintenance costs are assumed at 2% of capital expenditure.

3.5.2 Limitations of the Study

- I. Reformed Methanol HT-PEMFC System: The accuracy and applicability of the modelling/simulation to real-world application are limited by the following:
 1. Arrhenius-based kinetics is used for the reformer reactions, which do not consider complex catalyst behaviour or side reactions under varying conditions.
 2. Parameter uncertainty (literature-based values for Tafel slope, open-circuit voltage) may lead to potential inaccuracies in voltage and power predictions.
 3. Long-term degradation of the HT-PEMFC and reformer catalyst is not accounted for by the model, and these may reduce performance and efficiency over time.
 4. Simplification of model scaling(linear) from module to vessel-level neglects integration challenges (thermal management, gas distribution or stack interconnect losses).
 5. Auxiliary power demands are calculated as a fraction of simulated output power and may impact overall system efficiency.
- II. Comparative LifeCycle Analysis
 1. There is no dynamic variation of vessel operational conditions (e.g., speed variation, weather, engine loading factor, etc.), undermining real-world emission performance.
 2. Industrial and terrestrial datasets are used for extrapolation of emission factors, because of the limited availability of maritime-specific LCA data.
 3. Renewable electricity for e-methanol is assumed to be produced from fully decarbonised sources, undervaluing the authentic WtT emissions.
 4. The cradle-to-grave impacts of the conventional propulsion system are excluded from analysis, underrepresenting the total emission value.
- III. Techno-Economic Modelling
 1. Bio/e-methanol markets are still developing, making cost projections tentative.

2. Cost breakdowns do not account for balance-of-plant components (control units, heating and ventilation system, safety system, etc.).
3. Replacement costs of the HT-PEMFC subsystem are not modelled over the vessel's lifespan.
4. Risk premiums (insurance) and class certification costs for novel fuel systems are omitted from TCO calculations.
5. Interest rate fluctuations, inflation variability and exchange rate risk were not factored into the techno-economic modelling.

3.6 Summary

Comprehensive methodological framework for evaluating the feasibility of a methanol-fuelled HT-PEMFC for marine propulsion is evaluated herein. The methodology combines thermodynamic and electrochemical modelling, lifecycle analysis and economic evaluation. Key components include simulation of steam methanol reforming and HT-PEMFC stack performance using Python, scaling of module-level outputs to meet the propulsion demand of a Panamax-class vessel, comparative lifecycle analysis of GHG emission for vessel propulsion of conventional fuels and the methanol production pathways, and economic modelling of capital and operational cost, with sensitivity analysis to assess financial viability. The methodology is grounded in literature, validated against reference data, and designed to support decision-making for sustainable marine propulsion technologies. The results and interpretation of the simulations and analyses conducted will be presented in the subsequent chapters.

CHAPTER 4

OPERATING PERFORMANCE OF THE INTEGRATED SYSTEM– RESULTS AND DISCUSSION

4.0 Introduction

The reformed-methanol HT–PEMFC system offers a sustainable and efficient energy solution towards maritime decarbonisation and reduced emissions. A comprehensive analysis and discussion of the results obtained from the mathematical modelling of the system are presented in this chapter. Crucial knowledge of the system's kinetic, thermodynamic and electrochemical performance adapted for marine applications is simulated under specified operating conditions.

The MSR subsystem analysis elucidates the axial profiles of temperature, reactants, and products along reactor length, accentuating the interaction between heat transfer, endothermic reactions, and hydrogen permeation through a selective membrane. The impacts of varying steam-to-methanol ratio and inlet temperatures on methanol conversion, CO and CO₂ concentration, and hydrogen yield are explored through sensitivity analyses, guiding reformer efficiency optimisation while minimising undesirable by-products.

The key performance metrics for evaluating the HT–PEMFC system (stack voltage, power output, power density, and efficiency) as influenced by reformat gas parameters and the characteristic loss regimes (activation, ohmic and concentration) are illustrated in the simulated graphs. The overall integrated system efficiency over the range of power outputs is assessed to determine the optimal operating windows, with emphasis on its potential advantages in fuel utilisation and environmental impact compared to conventional marine diesel engines.

Waste-heat recovery and by-product management are superficially discussed, contextualising the viability of the system in real marine environments. This chapter

not only validates the fidelity of this model against literature and manufacturer data with these analyses but also identifies opportunities for improvement, paving the way for future experimental validation and system-scale deployment.

4.1 Methanol Steam Reformer Subsystem Model

The model was simulated to predict the species concentration, temperature distribution and performance metrics under specified inlet conditions (molar concentrations of reactants [methanol = 2500mol/m^3 , steam = 3750mol/m^3], $T_0 = 523.15\text{K}$ [250°C] and $P_0 = 1\text{atm}$). The results provide a comprehensive understanding of reformer behaviour under varying operating conditions.

4.1.1 Temperature Profile Along Reactor Length

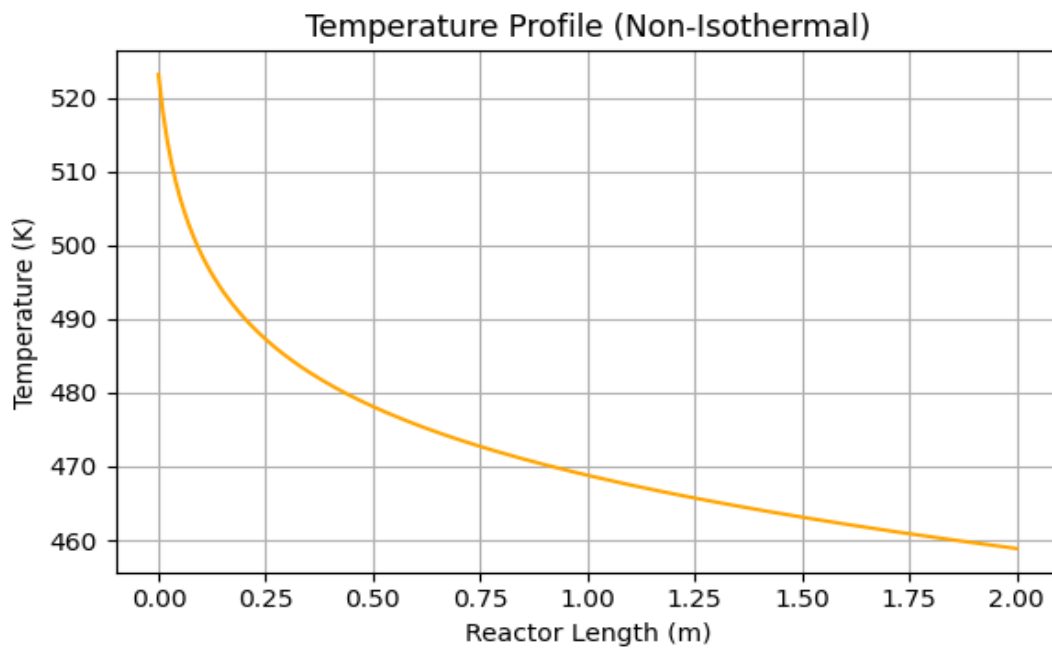
The distribution of temperature along the reactor length (figure 5) exhibits a slight increase at the inlet region (this is necessary to overcome the endothermic energy barrier of the steam reforming reaction), stabilising at the mid-section (aligning with optimal catalytic activity for Cu-based reformers, where methanol conversion efficiency and hydrogen selectivity are maximised) with a slight decline towards the outlet (resultant from heat losses, reaction equilibrium effects and competing exothermic WGS reaction).

The feed mixture (vapourised methanol-steam) enters the inlet section of the steam reformer at a pre-heated temperature— 523K (Zhuang et al., 2023). This temperature was chosen because it aligns with industry benchmarks, enhances proton conductivity and reaction kinetics, and enables efficient thermal integration without impairing membrane durability.

The effect of external heating causes a slight rise in the initial temperature at the beginning of the reaction process, aligning with the typical characteristics of SMR. Downstream from the inlet, the steam reforming reaction is vehemently endothermic, consuming heat rapidly and producing a noticeable temperature dip within 10–30%

(0.2–0.6m) of the reactor's length. The severity of the dip is dependent on feed preheat temperature, steam-to-carbon ratio, heat flux from heating medium and catalyst thermal conductivity (Rostami et al., 2023). This dip can be sufficient to reduce the reaction rate, requiring external heat input to prevent kinetic limitations (Li et al., 2023).

Figure 5: Temperature profile along reactor length at 523K



Source: Author

External heat from a furnace/jacket steadily offsets the endothermic load as the reaction progresses at the mid-section, causing a temperature recovery. This section of the reactor oftentimes represents a quasi-isothermal region, as the rate of heat supply matches the rate of heat consumption by methanol reforming and decomposition. Temperature stabilisation is crucial in this section to maintain a high rate of methanol conversion, as the reaction rate constant (k) increases exponentially with temperature according to Arrhenius law.

At the last 20–30% (1.5–2m) of the reactor length, most of the methanol had converted to products, and the reforming reaction approaches equilibrium with reduced reaction

heat demand. The slight drop in temperature at this stage is attributed to heat losses to the surroundings, and the decreasing rate of reaction as methanol concentration diminishes. Excessive heat is not supplied at this stage to avoid raising the outlet temperature excessively and promoting undesirable side reactions such as reverse WSG (RWSG), which causes high CO formation, although low outlet temperatures can result in incomplete conversion and low hydrogen yield; therefore, maintaining a sufficiently high outlet temperature (458K) is vital. The impact of varying inlet temperature is further explored in 4.1.5.

4.1.2 Reactant Species Profile

The overall kinetics, thermodynamics and product composition of the steam methanol reforming process are highly dependent on the selection and precise characterisation of the reactant species. The reactants (methanol and steam) serve primarily as carbon and hydrogen sources. Their molar proportions, purity levels, and phase properties directly influence hydrogen yield, catalyst performance and system stability. The reformer feed (reactants) composition highlighted in subsection 4.1 defines the steam-to-carbon ratio ($S/C=1.5$) and sets the starting partial pressures that determine initial reaction rates and thermodynamic driving force.

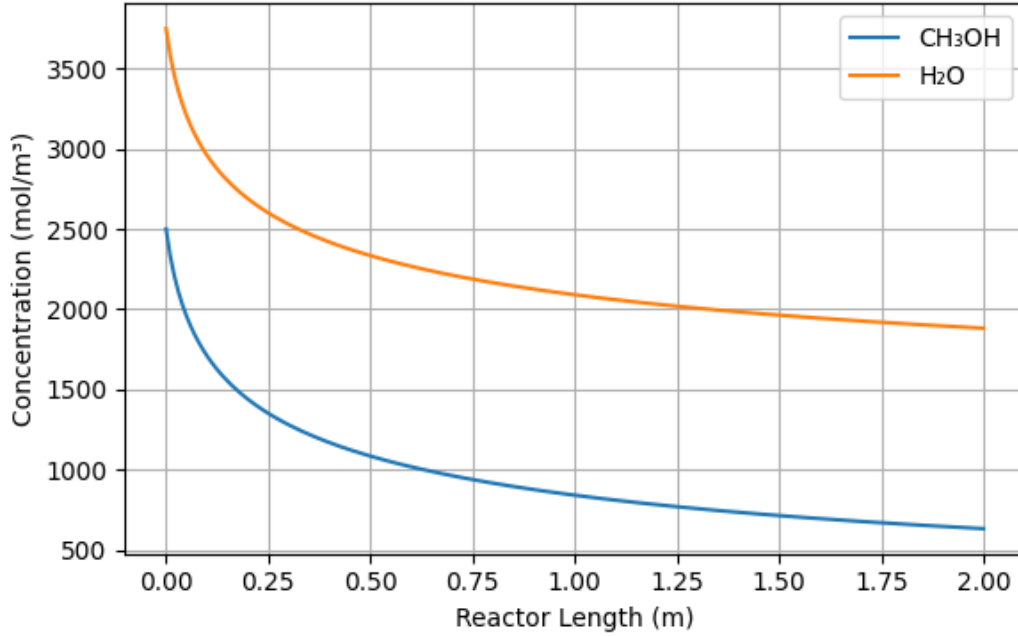
4.1.2.1 Properties of Reactant Species

Methanol is assumed to be 99.9% purity by volume (consistent with industrial-grade specifications for reforming applications). The choice of high-purity methanol ensures ideal reforming efficiency and extends catalyst lifetime, as minor impurities (higher alcohols, sulfur-containing compounds and aldehydes) poison the catalyst (Harkou et al, 2025; Rostami et al., 2023).

Water is supplied to the reformer as saturated steam at a pressure consistent with the reformer's inlet conditions. The steam quality is dry ($x=1$) as it promotes reliable heat transfer and prevents condensation within the feed lines (which could lead to localised cooling and incomplete methanol vaporisation). The steam is assumed to be pure without dissolved minerals or non-condensable gases, which may introduce side

reactions or scale formation on reformer surfaces. The reactants undergo thermal pre-conditioning (vaporisation by an evaporator) before entering the reformer to ensure phase compatibility (completely gaseous) and uniform mixing.

Figure 6: Reactant Concentration Profile at 523K



Source: Author

4.1.2.2 Axial Concentration Evolution

The reactant species configuration (Table 1) adopted for this study is impacted by mass transfer and membrane permeation. Localised methanol conversion at axial position (z) was computed as $\frac{C_{MeOH(i)} - C_{MeOH(z)}}{C_{MeOH(i)}} \times 100\%$, using $C_{MeOH(i)} = 2500 \text{ mol/m}^3$,

while localised S/C ratio was approximated by $S/C_{(z)} = \frac{C_{H_2O(z)}}{C_{MeOH(z)}}$. The local

methanol conversion and steam-to-methanol ratio in Figure 10 at respective axial positions show the following characteristic trends:

- Methanol concentration depletes steeply in the early axial section ($0 \rightarrow \sim 0.25 \text{ m}$) from 2500 to 1350 mol/m^3 due to high local reaction rates. This region

denotes a strong kinetic-control zone where high reactant partial pressures and elevated temperature drive local heat absorption (endothermic MSR and MD reactions), resulting in rapid hydrogen generation. High inlet methanol consumption implies intense localised endotherm; therefore, heat must be supplied fast in this region (multi-zone heating or high local heat flux is recommended to compensate for the solid endotherm at this region).

- ii. The concentration of steam decreases more gradually over the reactor length ($3750 \rightarrow 1853 \text{ mol/m}^3$). Steam is consumed by both SMR and WGS, causing its moderate decline over a longer distance, i.e., its axial gradient is shallower than methanol's. However, because steam was initially in excess ($S/C = 1.5$), the S/C ratio increases from 1.48 to 3.24 from the reactor inlet to the outlet. The downstream rise of the S/C signifies that methanol depletes faster than steam, helping to suppress CO formation by shifting the equilibrium towards WGS, but may result in excess steam generation affecting hydrogen selectivity. If steam consumption falls too low, it increases the risk of higher CO formation. The steady steam depletion downstream requires localised monitoring of the S/C ratio to prevent localised CO-formation, and if $S/C < 1$ at any point, a CO clean-up strategy or increased steam preheat is needed. An increased steam preheat temperature ensures that steam remains in the gaseous phase, preventing condensation and maintaining stable flow/reaction conditions, as well as providing additional thermal energy to drive endothermic reforming reactions, hence, enhancing hydrogen yield and suppressing CO formation.
- iii. Both reactants approach near-constant and low concentrations toward the outlet, as the conversion reaches its asymptote and reactions approach equilibrium. This is the region where residence time and simulated heat input cause a marginal increase in conversion (implying thermodynamic limits). To enhance conversion in this region, temperature elevation (whilst considering associated material and catalyst trade-offs), or longer reactor or enhanced hydrogen removal is required.

- iv. Hydrogen permeation is modelled as a flux to remove hydrogen along the reactor length, lowering local hydrogen partial pressure and thus shifting MSR and WGS equilibria forward (Le Chatelier effect). This practically enhances methanol conversion locally by scavenging hydrogen, ensuring a continuous reforming reaction. Membrane-permeation-assisted conversion indirectly reduces CO partial pressure (CO-producing reactions are suppressed when hydrogen is continuously extracted) and maintains CO within tolerable limits for fuel cell operation. However, an increase in permeation rate (P_{H2_perm}) results in increased energy penalty due to higher transmembrane pressure requirements (more membrane materials, potential compression or heating needs). Consequently, permeation rate [though not exclusively considered in this model] must be carefully optimised to maximise conversion and CO tolerance without incurring excessive energy or system complexity.

Table 1: Axial Concentration of Methanol and Steam

Axial Location [z] m	Methanol Concentration (mol/m ³)	Steam Concentration (mol/m ³)	Local S/C Ratio	Local Conversion (%)
0	2500	3750	1.5	0
0.25	1340	2591	1.93	46.40
0.5	1092	2332	2.14	56.32
1.0	844	2106	2.5	66.24
1.5	731	1982	2.71	70.76
2.0	580	1880	3.24	76.8

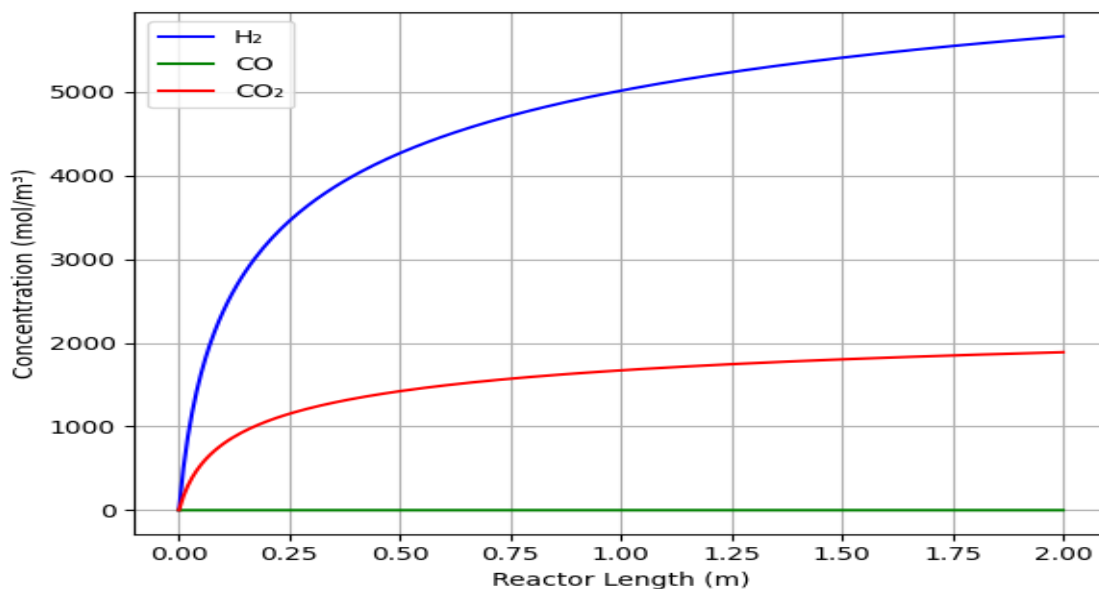
Source: Author

4.1.3 Product Species Profile

The primary objective of the reactor subsystem is hydrogen generation, which is evident in this simulation as hydrogen concentration increases along the reactor length with contributions from the three reactions. The reactants' concentration declines progressively along the reactor length as the those of the products (H₂, CO₂) increases,

suggesting effective reactant utilisation. Additionally, the methanol conversion efficiency and hydrogen purity are enhanced by integrating the reactor with a hydrogen-selective membrane.

Figure 7: Products Concentration Profile



Source: Author

Hydrogen generation begins speedily ($\sim 4300 \text{ mol/m}^3$) within the first 0.5m of the reactor length, as illustrated in Figure 7, driven primarily by the dominance of methanol steam reforming—where abundant reactant species produce 3 moles of hydrogen per methanol converted—and MD reactions. This increase plateaus after 1.0m, showing near-equilibrium conditions (limits further net production due to reactant depletion). This behaviour agrees with the MSR kinetic parameters (k_1 and E_{a1}), favouring high initial reaction rates at the inlet temperature. The selective removal of hydrogen [through the membrane] from the retentate stream shifts the equilibrium toward higher yields, with resultant total accumulation (retentate + permeate) of hydrogen supporting the observed plateau.

Conversely, CO₂ maintained a steep concentration gradient above 1000 mol/m^3 after its initial rapid rise (at 0.18m of reactor length), indicating a balanced production from MSR and WGS reactions without substantial accumulation. This profile suggests that

CO₂ formation is limited by upstream reactions and equilibrium shifts due to hydrogen removal. The intermediate conversion of CO to CO₂ while generating additional H₂ by the WGS reaction plays a vital role in modulating the CO₂ profile. The effectiveness of the WGS reaction in repressing CO [by rapid conversion to CO₂] is emphasised as the concentration of CO is notably negligible throughout (<2mol/m³). The kinetic parameters of the WGS reaction, its exothermic nature and excess inlet steam concentrations favour this repression. The low CO level is crucial for the downstream integration with the HT-PEMFC system.

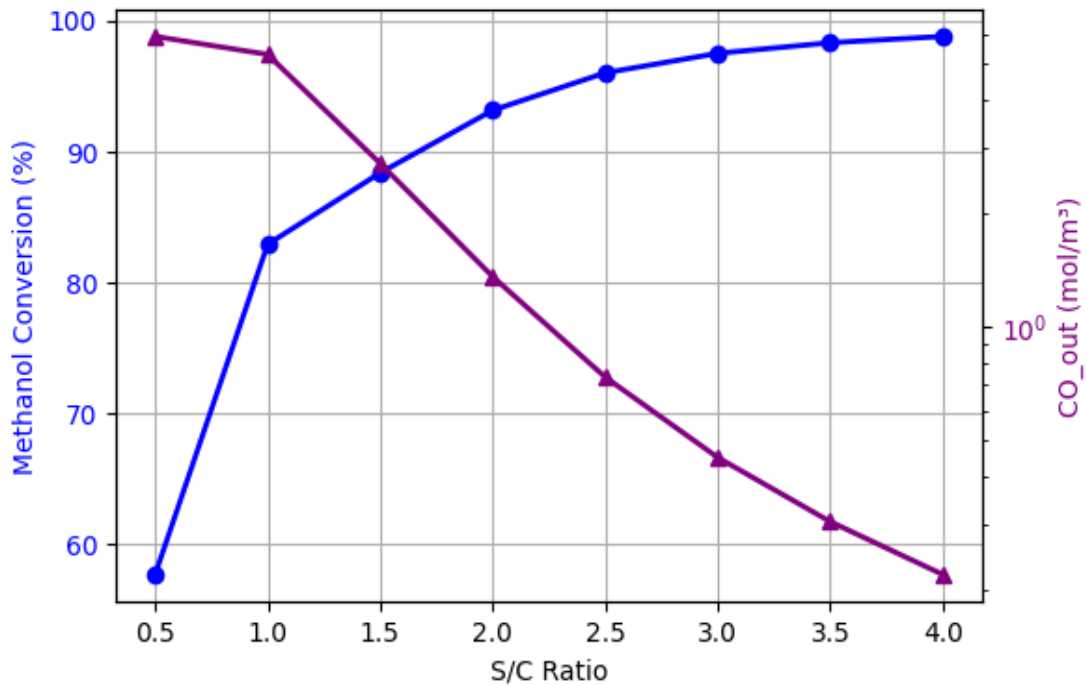
The product profile indicates a slightly efficient reformer operation (74.75% methanol conversion and ~74% hydrogen yield), consistent with the code's integrated metrics. The plateauing trends highlight potential limitations of reactant depletion and heat losses, while rapid hydrogen build-up and negligible CO indicate optimal conditions for feeding the HT-PEMFC.

4.1.4 Effect of Varying Inlet S/C Ratio on Methanol Conversion and Co Concentration

The influence of varying the initial S/C ratio (0.5–4.0) on methanol conversion and CO concentration is demonstrated in Figure 8, emphasising the effect of excess steam in shifting equilibrium and kinetics towards desired outcomes. At lower S/C ratios (0.5–1), conversion of methanol is constrained by the limited availability of reactant steam in the primary MSR pathway. Methanol conversion rises from 57.6% at an S/C ratio of 0.5 to almost 90% at S/C = 1.5 as steam availability increases, driving MSR forward and reducing unconverted methanol and CO in the product stream to generate more hydrogen [increased yield]. Methanol conversion further increases at an S/C >1.5, but approaches thermodynamic equilibrium. However, at S/C >2.5, conversion plateaus as the reaction reaches equilibrium constraints, and the benefits of excess steam become marginal. Further steam increase dilutes hydrogen by reducing its purity, requiring more heat for vaporisation.

At the lowest S/C ratio (0.5), CO production is highest, signifying the dominance of MD and limited WGS activity. CO concentration is noted to decline rapidly from 5.9mol/m^3 at $S/C = 0.5$ to 0.22mol/m^3 at $S/C = 4.0$, as higher steam quantity promotes WGS reaction. This suppresses CO formation, i.e., CO is rapidly converted to CO_2 , reducing its concentration to levels compatible with the HT-PEMFC system. These findings correspond to studies conducted by Chen et al. (2024), Chiu et al. (2019), and Park & Lee (2023).

Figure 8: Steam-to-Carbon Ratio Sensitivity Analysis at 523K



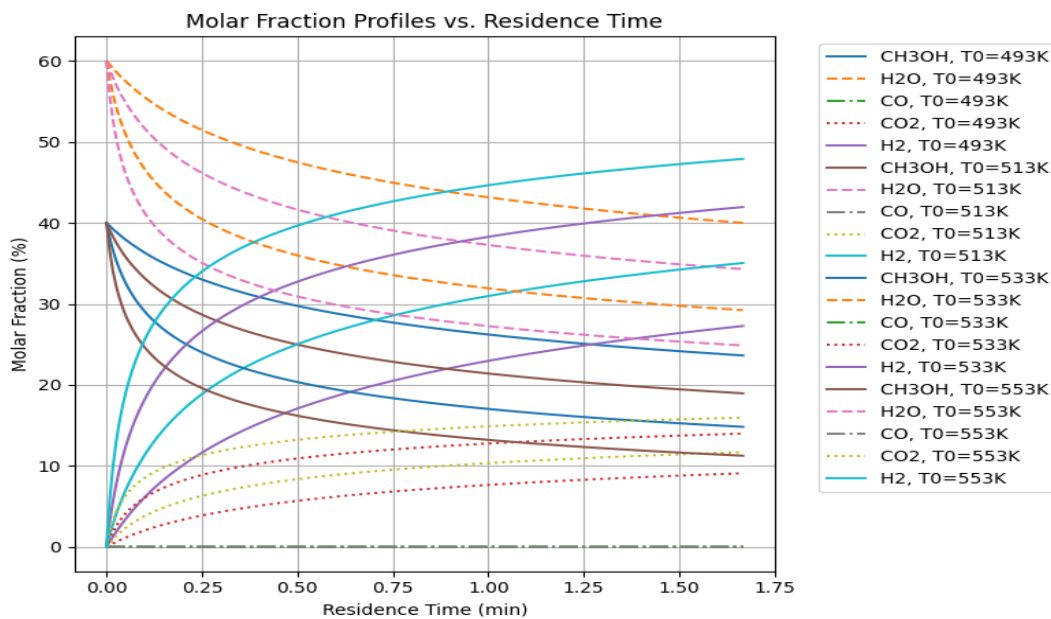
Source: Author

Substantially, S/C ratios > 1.5 optimise reformer performance (higher conversion, hence higher hydrogen yield, and lower CO), but with ratios ≥ 3 may impact hydrogen selectivity (dilution) and increase energy needed for vaporisation, implying an optimal S/C ratio of 1.5–2.0 for typical marine efficiency. Overall, this graph highlights the importance of optimising the S/C ratio for reformer designs to equilibrate thermal and energy requirements with the high methanol conversion (hydrogen yield) and negligible CO production.

4.1.5 Effect of Inlet Temperature on Methanol Reformer Performance

The initial inlet temperature, as a primary driver of reaction rates and equilibrium shifts in catalytic steam methanol reforming, determines the overall reaction kinetics and distribution of products. Elevated temperature ensures rapid methanol decomposition and steam reforming, thus accelerating hydrogen production in the initial stages. The simulation result (Figure 9) confirms that methanol conversion improves substantially as the inlet temperature increases. It can be deduced that the methanol molar fraction declines more rapidly along the reactor length at higher temperatures than at lower temperatures, showing that higher thermal input encourages more rapid and complete conversion of reactant species

Figure 9: Sensitivity Analysis of Inlet Temperature (at S/C = 1.5)



Source: Author

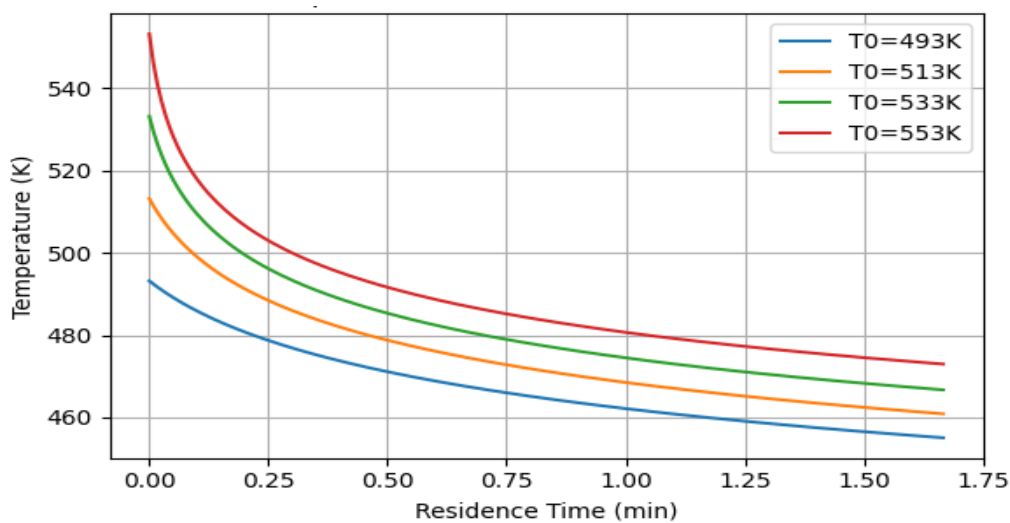
A strong positive correlation is also noted between inlet temperature and hydrogen yield. Higher inlet temperatures enhance both the MSR and MD pathways, resulting in increased hydrogen generation. At 553K, the molar fraction of hydrogen is remarkably higher than at lower temperatures (from 533K to 493 K), as thermal enhancement boosts conversion and shifts the equilibrium, favouring hydrogen production. This is an advantageous trend for fuel cell applications where critical performance metrics include hydrogen yield (availability) and purity. Rapid methanol

decomposition and increased hydrogen partial pressure are encouraged by high inlet region temperatures, while mid-region temperatures maintain selectivity towards hydrogen over CO and methane. However, at excessively high temperatures, side reactions such as methanation may occur; therefore, precise temperature control is essential to maintain the dominance of MSR, MD and WGS pathways over secondary reactions.

The production of CO₂ grows steadily with increasing inlet temperature, reflecting the combined effects of improved MSR and WGS reactions, which contribute to CO₂ formation. This steady increase in CO₂ molar fraction implies that greater thermal input boosts complete oxidation of carbon species, reducing the concentration of intermediate CO and improving reformer selectivity.

CO temperature dependency is complex as molar fractions increase with increased inlet temperature. However, at 553K, CO levels are noted to slightly drop owing to the increased activity of the WGS reaction, which converts steam and CO into H₂ and CO₂. This emphasises the significance of temperature control in curtailing CO slip, which is prejudicial to downstream FC integration.

Figure 10: Temperature Profiles versus Residence Time (at S/C = 1.5)



Source: Author

As seen in figure 10, temperatures below 513K have resultant waste heat below 160°C (low-grade), suitable for preheating of tanks or water vaporisation; but, operating temperatures of 513–553K can generate waste heat $160 \leq x \leq 230^\circ\text{C}$ (medium grade), which is transferred to support endothermic reactions such as MSR (Schuller et al., 2017). These findings, summarised in Appendix 5, accentuate the importance of precise thermal management in reformer design. This ensures that the heat supplied balances the endothermic demand without causing hotspots that may degrade the catalyst or cause uneven flow distribution, hence, optimising compatibility, selectivity and efficiency with FC systems.

4.2 HT–PEMFC Stack Subsystem Model

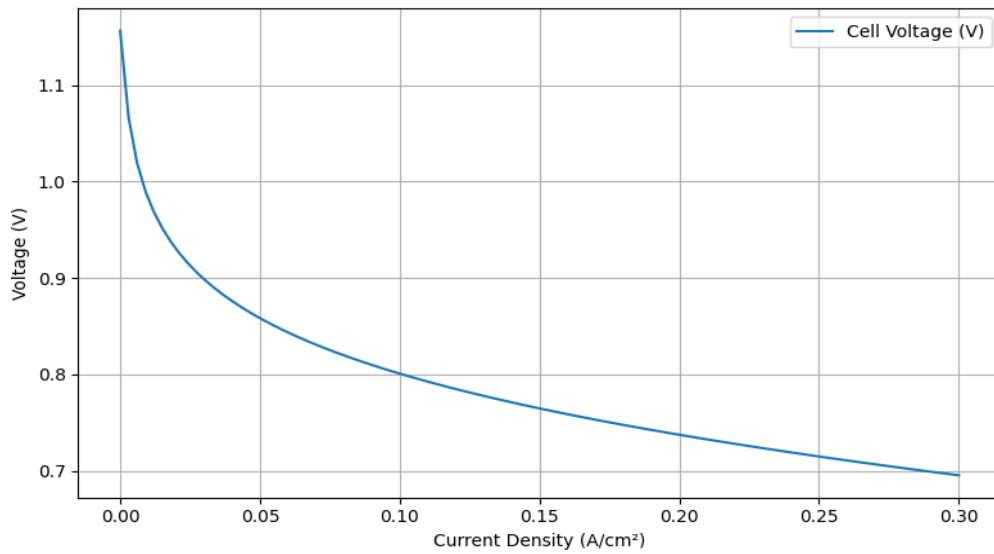
The model for the HT–PEMFC stack was developed to evaluate the electrochemical behaviour using the reformat gas from the Methanol Reformer. The configuration of the stack comprises 455 cells, each with an active area of 0.17m^2 (1700cm^2), operating at 160°C (433K) to coincide with high CO tolerance and the typical marine conditions that prioritise thermal stability. Some key parameters are an open–circuit voltage ($E_0 = 1.13\text{V}$), exchange current density ($j_0 = 1.2\text{e-}3$), ohmic resistance ($R_{\text{ohmic}} = 0.1\Omega.\text{cm}^2$) and limiting current density ($j_{\text{lim}} = 1.3\text{A}/\text{cm}^2$). To ensure that the current stack remains below 500A (maxing out at $\sim 500\text{A}$), reflecting realistic operational limits and avoiding overpotentials, the current density range (j_{range}) was set from $0\text{--}0.3\text{A}/\text{cm}^2$. These parameters enable stack power outputs of approximately 160kW. This section evaluates stack voltage, power, efficiency and the integrated system efficiency, comparing it to a manufacturer's datasheet for validation.

4.2.1 Stack Voltage and Power Characteristics

The typical three–regime behaviour of PEM fuel cells is exhibited by the polarisation ($V\text{--}j$) curve for cell voltage versus current density (Figure 11). These regimes are activation–domination at low densities ($0\text{--}0.05\text{A}/\text{cm}^2$), ohmic–domination in the mid–range ($0.05\text{--}0.2\text{A}/\text{cm}^2$) and concentration–limitation at higher densities ($> 0.2\text{A}/\text{cm}^2$). The OCV starts from 1.13V, but voltage declines curvilinearly to $\sim 0.72\text{V}$ at $0.3\text{A}/\text{cm}^2$.

Activation overpotentials contribute to the initial drop (solved by Butler–Volmer equation), as j_0 requires significant overpotential to initiate hydrogen oxidation and oxygen reduction (Redox) reactions. The ohmic losses from ionic and electronic resistances in the PBI membrane and bipolar plates transit to a quasi–linear slope. Concentration overpotentials accelerate the decline of reactant diffusion limits to approach j_{lim} at higher densities.

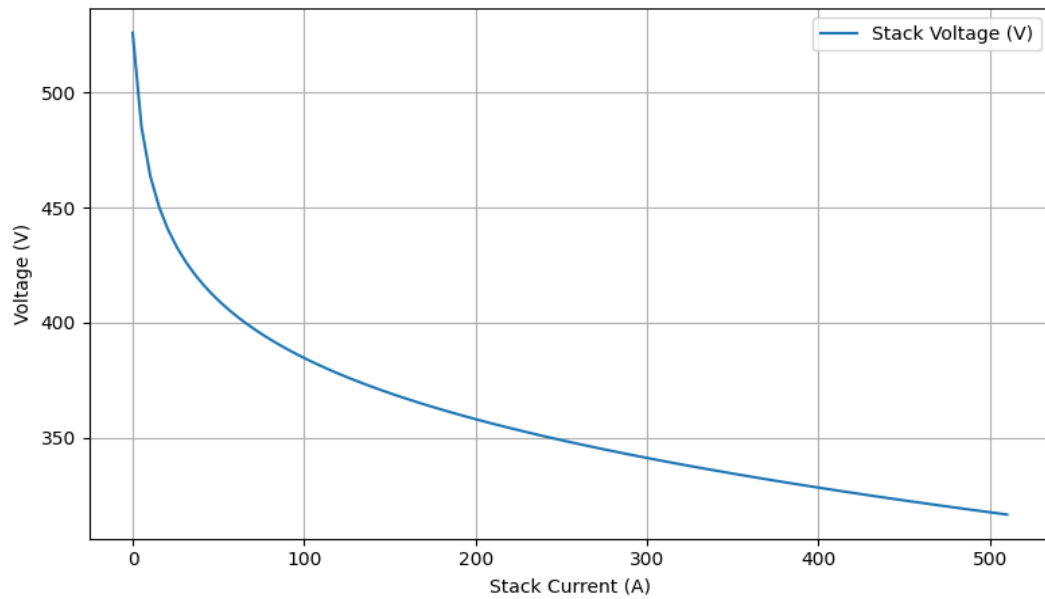
Figure 11: Cell Voltage versus Current Density



Source: Author

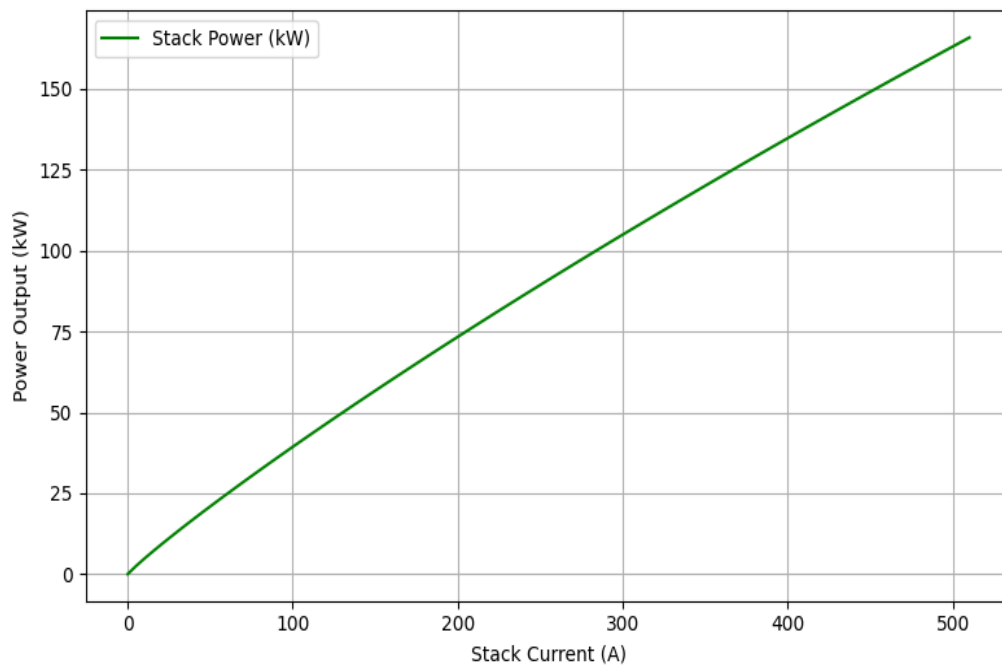
The Nernst–calibrated OCV exceeds standard E_0 because of the beneficial hydrogen partial pressure from the reformat stream. E_{Nernst} reaches 1.17V with resultant initial $V_{cell} \approx 1.13V$. This reflects improved thermodynamic driving force under non–standard conditions and is physically valid. A voltage yield of 517.5V at OCV and scaled by n_{cells} to 325.7V at 500A, suitable for direct DC propulsion motors, is illustrated in the polarisation curve (Figure 12).

Figure 12: Polarisation Curve



Source: Author

Figure 13: Power–Current Graph

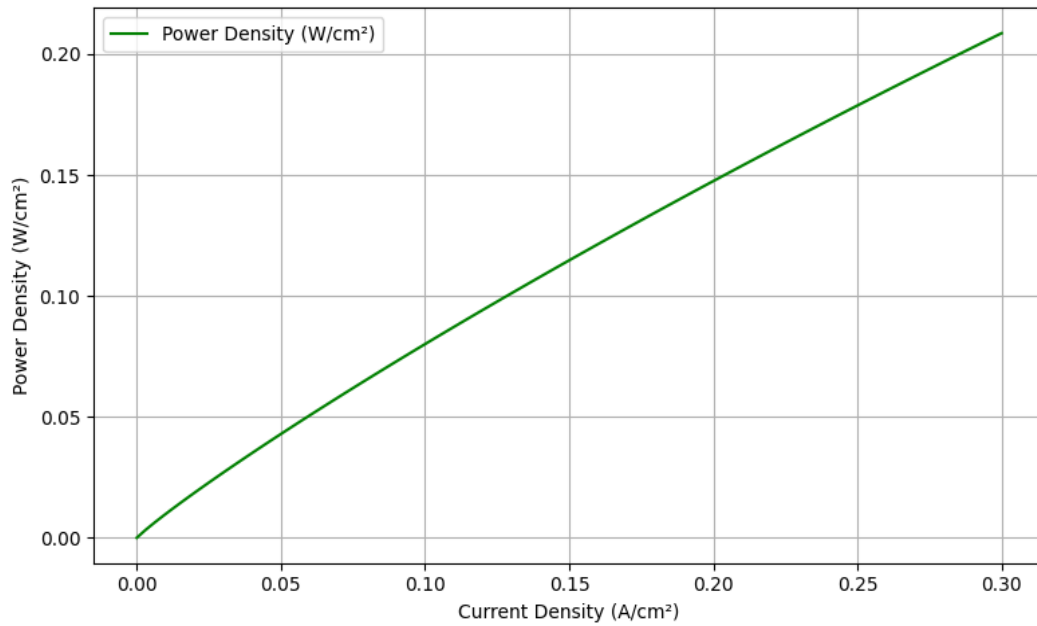


Source: Author

A power of ~160kW near 500A reflects the voltage–current trade-off seen in Figure 13; this corresponds to the validation noted in Chapter 3.3.4. Power density reaches

$\sim 0.22 \text{ W/cm}^2$ at a current density of 0.3 A/cm^2 (figure 14). This model's fidelity is validated [through extrapolation] by Ballard (2025) marine PEMFC datasheets (targeted $0.3\text{--}0.5 \text{ W/cm}^2$ for 200kW modules). Discrepancies in this model are due to optimised reformate composition and reduced ohmic losses, underscoring ideal marine operations with efficient cooling.

Figure 14: Power Density versus Current Density Graph

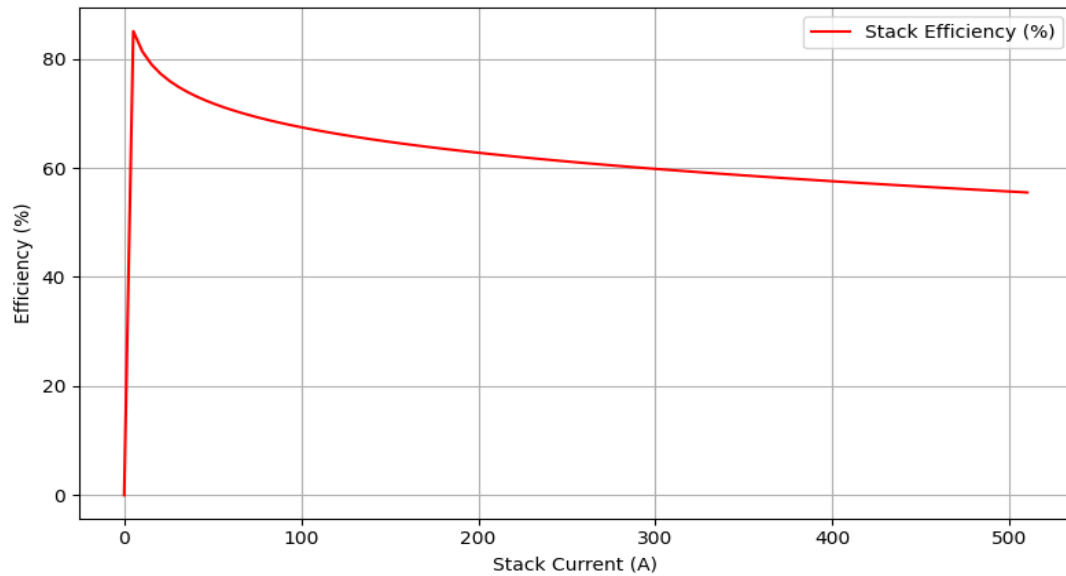


Source: Author

4.2.2 Stack Efficiency

Stack efficiency (figure 15), the ratio of electrical P_{output} to hydrogen LHV input, decreases from $\sim 80\%$ at low current to $\sim 56\%$ at 500A. This trend signifies increasing overpotentials; initial activation loss dominance reduces efficiency by 10–15%, with ohmic and concentration losses noted at higher currents. Steep initial drop accompanied by a gradual decline is archetypal of HT-PEMFC with PBI membranes. This model shows higher peak efficiency ($\sim 80\%$) versus Zhuang et al.'s (2023) ($\sim 50\%$), consequent to the discrepancies in section 4.3.1; however, overall decline corresponds with a 10–15% drop over a similar range.

Figure 15: Stack Efficiency Graph



Source: Author

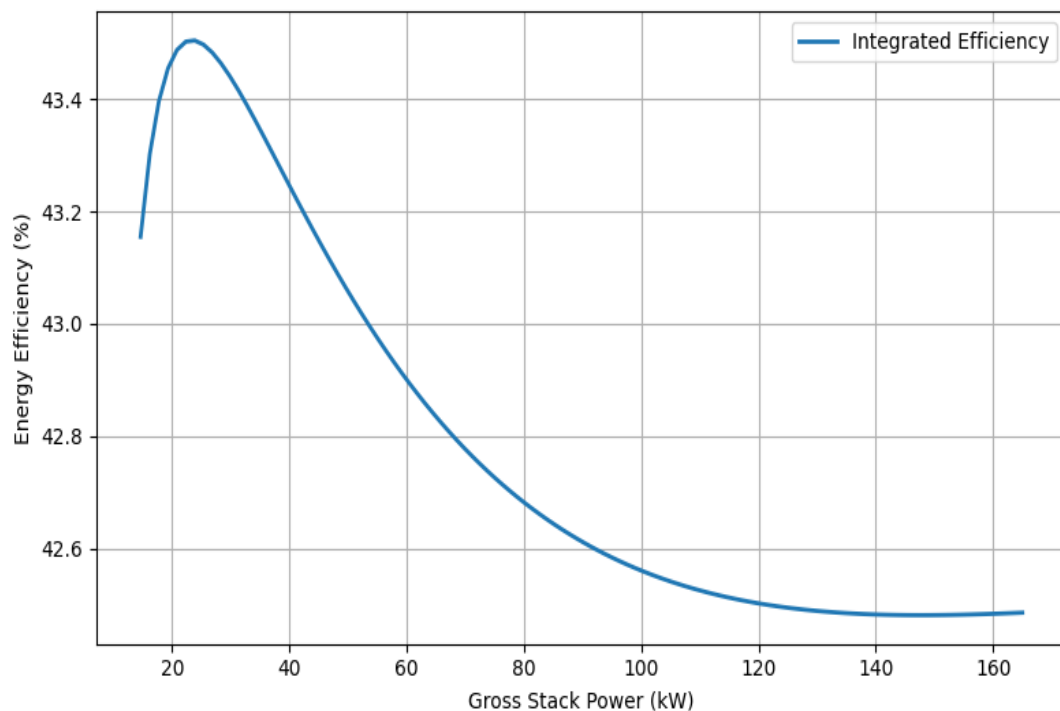
4.2.3 Efficiency of Integrated System

The integrated system efficiency (figure 16) is characterised by a non-linear trend vis-à-vis the stack output power. Peak efficiency (~43.35%) is achieved at 25.6kW as seen in the simulation result, corresponding to the optimal operating point of thermally and kinetically balanced reformer and HT-PEMFC subsystems. Increased methanol conversion and maximised hydrogen yield are noted at this stage, with the HT-PEMFC stack operating at its most favourable electrochemical regime (minimal activation and ohmic losses, stable reactant flow).

A gradual decline is noted after the optimal range as efficiency falls to ~42.46% at 160kW, attributed to several interrelated factors. Heat and mass transport limitations are encountered at the reformer subsystem at this stage, constraining methanol conversion and hydrogen production. Maintaining uniform temperature distribution and mixing of reactants becomes challenging as throughput increases, resulting in localised inefficiencies and reduced hydrogen purity. Concurrently, there is intensified ohmic and concentration overpotentials at higher power outputs as fuel cells

experience increased current densities. These losses consequently reduce effective cell voltage and electrical efficiency. Additionally, energy consumption of auxiliary components (parasitic losses) scales upwards with power output, further diminishing net system efficiency. When compared with conventional marine diesel engines—typical maximum efficiency of ~40%—this integrated system achieves slightly stronger benchmarks (which declines with higher power outputs) and remarkably lower emissions when operated within its optimal efficiency window. This weakness may partially explain their inability to surpass ICE technology in large-scale applications.

Figure 16: Efficiency of Integrated System



Source: Author

For maritime propulsion applications characterised by dynamic load profiles, this efficiency trend implies that the integrated system performs best under partial load (specifically 20–100kW range). Operating within this range optimises fuel utilisation and improves thermal management. Contrarily, there may be increased fuel consumption and reduced economic viability because of lower energy conversion

efficiency and higher auxiliary demands. This emphasises the importance of system sizing and strategic load management for fuel cell integration in maritime propulsion.

4.2.4 Waste Heat Recovery, Water and By-products Management

The reformer contributes supplementary heat through endothermic reactions and latent heat requirements, which sustain reaction kinetics. The operating temperature of the HT-PEMFC system proffers notable potential for waste heat recovery in maritime applications where thermal integration enhances overall system efficiency. Losses (activation, ohmic and concentration) convert 50–60% of input chemical energy to heat within the fuel cell stack. The low-grade thermal energy will be recovered and redirected via a liquid circuit for preheating reactant feedstock and maintaining vaporisation conditions of reformer and FC humidifier, reducing external energy demands (electric heaters or combustion burners). This enhances fuel utilisation and improves integrated system efficiency (Schuller et al., 2017).

The by-products of the MSR system are CO₂ and trace amounts of CO (whose prolonged exposure degrades the performance of HT-PEMFC). Water vapour and heat are the by-products of the HT-PEMFC system. To ensure regulatory compliance, CO₂ will be sequestered onboard, while trace CO will be significantly reduced by Preferential Oxidation (PROX) units, increasing the overall cost of the system.

Phosphoric acid-doped polybenzimidazole membranes in HT-PEMFC simplify the system design by eliminating the need for external humidification. Water vapour produced from HT-PEMFC operation is typically vented with exhaust gases. For long-range vessels, water recovery systems (condenser/gas-liquid separators) although this incurs extra cost and energy demand, may be utilised to condense water for subsequent reuse to feed the reformer or cooling circuits, minimising freshwater consumption and supporting sustainable operations.

CHAPTER 5

ENVIRONMENTAL AND ECONOMIC ANALYSIS–RESULTS AND DISCUSSION

5.0 Introduction

Elaborating on the operational practicability discussed in Chapter 4, the following analysis explores the environmental and economic performance of the integrated system, satisfying research objectives on lifecycle GHG emissions and financial viability. A cradle-to-grave lifecycle assessment compares methanol-based propulsion technologies to conventional propulsion systems (HFO, MGO) on the following metrics: absolute savings, daily avoidance, decadal mitigation and sensitivity to emission factors. Furthermore, a complementary techno-economic assessment evaluates the total cost of ownership (TCO), levelized cost of energy (LCOE), and discounted payback periods under market-driven (baseline) and policy-driven scenarios. This is reinforced by Monte Carlo uncertainty simulations on CAPEX, efficiencies and fuel prices; evaluating risk profiles and confidence intervals.

5.1 Lifecycle Analysis

This sub-section critically evaluates the environmental [GHG] performance of a 6MW integrated MSR and HT-PEMFC system for a Panamax-classed vessel gauged against conventional marine engines. A cradle-to-grave approach based on ISO 14040/14044 standards is adopted for this analysis, comprising manufacturing, operational ([WtT] and [TtW]) and End-of-Life (EOL) phases. Key assumptions from Nyanya et al. (2021) include conventional engine $P_{\text{output}} = 6100\text{kW}$, DWT = 80,000, daily fuel consumption = 40tonnes, loading factor = 70%, average operational speed = 14knots, operational days/year = 250, and operational lifetime = 25years. For simplicity and time constraints, variability from load profiles and maintenance emissions is excluded. Methanol consumption is scaled from code-derived values (68.2tonnes/day at ~42.5% integrated system efficiency).

LCA findings are synthesised in this discussion, underscoring the system's decarbonisation potential for maritime propulsion. The subsequent analysis quantifies emission as: absolute[lifetime] emission savings (tCO₂eq), relative emission reductions (%), daily emission avoidance and decadal mitigation potential. The primary baseline (HFO) is dominant in conventional shipping, while MGO is included for robustness.

5.1.1 Manufacturing Phase

The manufacturing emission (WtT) for this discussion is calculated by multiplying the emission factors (kgCO₂eq/kg.material) by the required material quantity (kg) for the modelled design (HT–PEMPC subsystem only for simplification). The quantities of component materials are tabulated in Appendix 6. The emissions from material extraction to production are obtained from the Life Cycle Inventory (LCI) database – EcoInvent (v3.8). The quantity of methanol consumed for the scaled output power is calculated based on the integrated system efficiency (~42.5% at 160kW) at steady–state operation to determine the daily operational emission.

$$\text{Methanol energy input} = \frac{\text{Net Power}_{\text{output}}}{\eta_{\text{integrated}}} = \frac{160}{0.425} = 376.47\text{kW} \text{ (376,470J/s)}$$

$$\text{Methanol consumption rate} = \frac{\text{Energy}_{\text{input}}}{\text{LHV}_{\text{MeOH}}} = \frac{376470}{638000} = 0.59\text{mol/s}$$

$$\text{Methanol mass flow rate} = \text{consumption rate} \times \text{molar mass}_{\text{MeOH}} = 0.59 \times 0.032 = 0.0189 \text{ kg/s } (\times 3600 \text{ sec/hr}) = 67.98\text{kg/hr}$$

$$\text{Specific Methanol Consumption} = \frac{\text{Mass flow rate}}{\text{Power}_{\text{output}}} = \frac{67.98}{160} = 0.425\text{kg/kWh}$$

Apparently, 68kg of methanol is required to produce 160kW output power for an hour, and 1794.67kg for 24hours (factoring 5–10% for variable loads and degradation). A 6MW–output power translates to $1794.67 \times 38\text{modules} = 68,197\text{kg} \approx 68.2\text{tons/day}$.

- Material Production emission: PBI (10.61kg x 8.8) + CL (0.65kg x 3.34 x10⁴) + GDL (19kg x N/A)¹ + Bipolar plates (232kg x 5.34) + Seals (2.32kg x 5.34) + End plates (84kg x 5.13) = 23,054.5kgCO₂eq = 23.05tCO₂eq
- For the referenced Panamax vessel, 38 modules are required to produce the net power output and the equivalent emission from material production = 38 x 23.05 = 875.9tCO₂eq.
- Transportation: Shipping of components from Japan to manufacturers, and from manufacturers to shipyard (China) (~29484n.miles) and road transport (~704km) has estimated emissions of 6.94tCO₂eq as extrapolated from Table 2.

Table 2: Transport Energy Consumption and CO₂ Footprint

	Energy (GJ)	CO ₂ (t)
Transport Case road 200 km	2.94	0.21
Transport Case road 2593 km	38.17	2.71
Transport Case sea 600 nautical miles	1.78	0.13
Transport Case sea 13471 nautical miles	39.92	2.83

Source: Liu & Barlow, 2017

Total emission from manufacturing phase = 875.9 + 6.94 = **882.84tCO₂eq**

For a single 160kW HT-PEMFC module, manufacturing emissions totalled 23.05tCO₂eq. The scaled 6MW amounted to 882.84tCO₂e (dominated by precious metals' high impact from mining intensity and composites), with 99% from material extraction and production and <1% from transportation (Liu & Barrow, 2017).

5.1.2 Operational Phase

5.1.2.1 Upstream Emission (WtT)

This subsection discusses the upstream (production and supply chain) emissions generated from the various methanol pathways required for the vessel's daily power

¹ Where data is not available, emission generated equals 0.

(approximately 6MW). Emission factors used are mid-point averaged from literature ranges and summarised in Table 3.

Table 3: Emission ranges of the Fuel Options

S/N	Fuel	Emission Factor Well-to-Wake (gCO ₂ eq/MJ)	Energy Density [LCV] (MJ/g)	Emission Factor Well-to-Wake (gCO ₂ eq/gFuel)	Midpoint Average (gCO ₂ eq/gFuel)
1.	Grey methanol [WtT]	103 – 110	0.0199	2.0 – 2.2	2.1
2.	Blue methanol [WtT]	91.6 – 101	0.0199	1.82– 2.01	1.91
3.	E-methanol [WtT]	0.22 – 7.64	0.0199	0.0044 – 0.15	0.077
4.	Bio-methanol [WtT]	-120 – 55	0.0199	-2.388 – 1.095	-0.647
5.	HFO [WtW]	94.26	0.0402	0.675 (WtT) + 3.114 (TtW)	3.789
6.	MGO [WtW]	92.78	0.0427	0.756 (WtT) + 3.206 (TtW)	3.962

Source: Methanol Institute (2023), IMO (2024)

Midpoint averaging is used for methanol pathways to derive point estimates for a simplified comparison while reflecting typical operational conditions and current technological baselines. Upper and lower bounds of the emission ranges are explored via scenario analysis to address the variability of fuel production pathways. Baseline fuels use WtT, TtW, and WtW values as applicable.

Table 4: Upstream Emissions of the Fuel Options

Fuel Pathway	Emission Factor (avg.) (tCO ₂ eq/tFuel)	Methanol Quantity (ton/day)	Daily Emission (tCO ₂ eq)	Yearly Emission [250days/year] (tCO ₂ eq)	Lifetime Emission [25years] (tCO ₂ eq)
Grey Methanol	2.1	68.2	143.22	35,805	895,125
Blue Methanol	1.91	68.2	130.26	32,565.5	814,137.5
Bio-Methanol	-0.647	68.2	-44.13	-11,031.35	-275,783.75
E-Methanol	0.077	68.2	5.25	1,312.85	32,821.25
HFO (WtT)	0.675	40	27	6,753.6	168,840
MGO (WtT)	0.756	40	30.24	7,560	189,000

Source: Author

Table 4 illustrates the upstream emission profiles of the fuels. Grey methanol's daily amount (143.22tCO₂eq) reflects fossil-based synthesis, demonstrating its decarbonisation unsuitability, as HFO/MGO has lower values. Blue methanol is slightly lower due to carbon capture and recirculation, but depends on capture efficiency and methanol leakage. Bio-methanol demonstrates a net-negative (-44.13tCO₂eq) emission value due to biogenic carbon [sequestration] credits, i.e., plants absorb atmospheric CO₂ during growth, approximately balancing out the tank-to-wake phase; and e-methanol is significantly lower (5.25tCO₂eq) but highly sensitive to electricity (renewable or grid-mix) and CO₂ input requirements.

5.1.2.1.1 Sensitivity Analysis on Emission Factor Range

Dependence on feedstock, technology and energy inputs demonstrates substantial variability in the emission of methanol production pathways based on this scenario analysis (Table 5). Grey methanol accounts for the highest emission, serving as the baseline, with its lifetime emissions range highlighting the transformational potential of renewable pathways. Blue methanol (~10% <grey) shows CCS's mitigation potential, although its high scenario overlaps with grey's low scenario, highlighting dependency on CCS efficiency. Bio-methanol exhibits the best mitigation potential under sustainable sourcing, although land-use pressures may induce reversal risks. E-methanol poses as a near-zero solution, although grid-mix may inflate emission values.

Table 5: Emission Ranges Scenario Analysis

PRODUCTION PATHWAY	SCENARIO	EMISSION FACTOR tCo2eq/tFuel	DAILY EMISSION	YEARLY EMISSION	LIFETIME
			tCO2eq		
GREY METHANOL	LOW	2	136.4	34100	852500
	BASE	2.1	143.22	35805	895125
	HIGH	2.2	150.04	37510	937750
BLUE METHANOL	LOW	1.82	124.124	31031	775775
	BASE	1.91	130.262	32565.5	814137.5
	HIGH	2.01	137.082	34270.5	856762.5
BIO-METHANOL	LOW	-2.38	-162.316	-40579	-1014475
	BASE	-0.647	-44.1254	-11031.35	-275784
	HIGH	1.095	74.679	18669.75	466743.8
E-METHANOL	LOW	0.0044	0.30008	75.02	1875.5
	BASE	0.077	5.2514	1312.85	32821.25
	HIGH	0.15	10.23	2557.5	63937.5

Source: Author

Bio- and E-methanol pathways align with IMO's targets, although bio-methanol's high value might experience rebound effects from biomass competition. Renewable pathways demonstrate transformative potentials, but scenario analysis did not factor in policies, energy mix and supply chain dynamics, which influence outcomes. The viability of low-emission pathways could considerably improve with economic incentives; however, further assessment of full lifecycle impacts (land, water and energy use) is crucial.

5.1.2.2 Downstream Emission (TtW)

Direct combustion of fossil fuels typically dominates GHG profiles in downstream analysis. The conventional fuels, HFO yielded 31,140tCO₂/year and 778,500tCO₂e over an operational lifespan, while MFO resulted in 32,060tCO₂/year and 801,500tCO₂e/lifetime as seen in Table 6.

Table 6: Conventional Fuels Emission Profile

S/N	Conventional Fuel	Daily Fuel Consumption (tons)	Emission Factor (tCO ₂ e/t.Fuel)	Daily Emissions (tCO ₂ eq)	Yearly Emission [250days/year] (tCO ₂ eq)	Lifetime Emission [25years] (tCO ₂ eq)
1.	HFO	40	3.114	124.5	31,140	778,500
2.	MGO	40	3.206	128.24	32,060	801,500

Source: Author

However, downstream emissions from the integrated system are not discussed as CO₂ generated from MSR operation is assumed to be sequestered. Due to the intricacy of the reactor size, energy demands, efficiency of the CCS system and storage/offloading logistics and for simplified discussion, calculation of the emission intensity based on the quantity of CO₂ emitted and captured, and net power output is omitted in this discussion and downstream integrated system emission is assumed to be negligible. This exclusion potentially underestimates lifecycle emissions because if CCS efficiency significantly drops (<90%), the system's net climate impact could be materially affected.

5.1.3 End-of-Life (EOL) Phase

The EOL Phase presents material recovery and recycling credits offering substantial offsetting opportunities, with predominant metal recovery (valuable and energy-intensive materials, e.g., stainless steel, platinum), compensating primary production impacts from lifecycle emissions. The net recycling credit (Table 7) for ~160kW HT-PEMFC system is **-22.169tCO₂e**, extrapolated for a 6MW(**-842.42tCO₂e**), reflects avoidable virgin material production and landfill disposal emissions. Various caveats are acknowledged for this phase: recycling processes are energy-intensive and dependent on regional capabilities, and should be accounted for in LCA, market demand for secondary materials, and regulatory frameworks. The recycling credits (Appendix 7) for platinum was obtained from CORDIS (2020), while 87% for the other materials was adopted from OECD (2019).

Table 7: Recycling Credits

S/N	Material	Emission factors (WtT) (kgCO ₂ e/kg)	Recycling Rate (%)	Material Quantity	Recycling Credit (kgCO ₂ e)
1.	Polybenzimidazole (PEM)	8.87	87	10.61	81.88
2.	Platinum (catalyst layer)	33400	95	0.65	20624
3.	Carbon cloth (gas diffusion layer)	N/A	-	19	-
4.	Graphite composites (bipolar plates)	5.34	87	232	1077.83
5.	Graphite composites (seals/gaskets)	5.34	87	2.32	10.78
6.	Stainless alloy (end plates)	5.13	87	84	374.9
Recycling Credit (for one 160kW module)					22,169.88
Total Recycling Credit (for 6MW, i.e., 38 modules of 160kW)					842,455.44

Source: Author

The importance of design-for-recyclability in future HT-PEMFC systems is buttressed by the EOL phase. Materials with recovery pathways and minimised composite complexity enhance circularity and reduce lifecycle emissions. EOL integration into procurement and maintenance strategies improves cost-effectiveness and regulatory compliance. HT-PEMFCs are part of a closed-loop maritime energy strategy, minimising emissions across the entire material lifecycle.

Table 8: Summary of Emissions on MSR-HT–PEMFC Scenarios Versus Conventional Alternatives

Life-Cycle Phase	MSR + HT-PEMFC with Grey Methanol (tCO ₂ eq)	MSR + HT-PEMFC with Blue Methanol (tCO ₂ eq)	MSR + HT-PEMFC with Bio-Methanol (tCO ₂ eq)	MSR + HT-PEMFC with E-Methanol (tCO ₂ eq)	Conventional HFO Engine (tCO ₂ eq)	Conventional MGO Engine (tCO ₂ eq)
Upstream (Lifetime)	896,007.84	815,020.34	-274,900.91	33,704.09	168,840	189,000
Operation (Lifetime)	N/A i.e., 0	N/A i.e., 0	N/A i.e., 0	N/A i.e., 0	778,500	801,500
End-of-Life	-842.42	-842.42	-842.42	-842.42	N/A i.e., 0	N/A i.e., 0
Total (Lifetime)	895,165.42	814,177.92	-275,743.33	32,826.09	947,340	990,500

Source: Author

This summary (Table 8) demonstrates that the use of bio-methanol and e-methanol pathways is environmentally advantageous, reflecting lifecycle modelling that warrants closer examination. However, bio-methanol's negative emission values are dependent on key assumptions, including the use of sustainable and renewable biomass that does not induce land-use change, effective capture and sequestration of process emissions permanently stored in geological formations, and low-carbon energy inputs. Similarly, e-methanol's low value stems from the assumption that it is synthesised from green hydrogen (i.e., electrolysis using renewable electricity) and CO₂ from biogenic or industrial sources. These assumptions are contingent on exclusive use of renewable electricity in the supply chain and consistent high-efficiency CO₂ capture. The climatic advantage diminishes if assumptions are not met, as it remains sensitive to feedstock availability, carbon accounting boundaries and upstream energy inputs, limiting sustainability.

5.1.4 Comparative Emission Metrics

Methanol production pathways are comparatively assessed against conventional marine fuels across the emission metrics in Table 9. This analysis provides a quantitative lens for evaluating the climate efficacy of each pathway for maritime decarbonisation. The absolute emission savings are calculated as $(lifetime\ emission_{baseline} - lifetime\ emission_{methanol\ pathway})$, while the relative emission reduction is calculated from the emission intensity of the transport work $\left(\frac{emission\ intensity_{baseline} - emission\ intensity_{methanol\ pathway}}{emission\ intensity_{baseline}}\right) \times 100$. Daily emission avoidance is calculated as $(daily\ emissions_{baseline} - daily\ emissions_{methanol\ pathway})$, and decadal mitigation $((yearly\ emissions_{baseline} - yearly\ emissions_{methanol\ pathway}) \times 10)$.

Transport work calculation: annual transport work = $80,000\text{DWT} \times 70\%$ (loading factor) $\times 250$ sailing days $\times (14\text{knots} \times 24\text{hrs}) = 4.704 \times 10^9$ tonne-miles.

Lifetime transport work = $4.704 \times 10^9 \times 25\text{years} = 11.76 \times 10^{10}$ tonne-miles.

Emission Intensity of the alternatives:

HFO–Conventional = $947,340 \div (11.76 \times 10^{10}) = \mathbf{8.05gCO_2eq/ton.mile}$

MGO–Conventional = $990,500 \div (11.76 \times 10^{10}) = \mathbf{8.42gCO_2eq/ton.mile}$

Grey–Methanol = $895,165.42 \div (11.76 \times 10^{10}) = \mathbf{7.61gCO_2eq/ton.mile}$

Blue–Methanol = $814,177.92 \div (11.76 \times 10^{10}) = \mathbf{6.92gCO_2eq/ton.mile}$

Bio–Methanol = $-275,743.33 \div (11.76 \times 10^{10}) = \mathbf{-2.34gCO_2eq/ton.mile}$

E–Methanol = $32,826.09 \div (11.76 \times 10^{10}) = \mathbf{0.28gCO_2eq/ton.mile}$

Table 9: Comparative Performance of Emission Metrics

S/ N	Emission Metrics	Baseline	Grey Methanol	Blue Methanol	Bio– Methanol	E–Methanol
1.	Absolute Emission Savings (tCO ₂ e)	HFO	52,174.58	133,162.08	1,223,083.33	914,513.91
		MGO	95,334.58	176,332.08	1,266,243.33	957,673.91
2.	Relative Emission Reduction (%)	HFO	5.47	14.04	129.07	96.52
		MGO	9.62	17.81	127.79	96.67
3.	Daily Emission Avoidance (tCO ₂ e/day)	HFO	8.28	21.24	195.63	146.25
		MGO	15.26	28.22	202.61	153.23
4.	Decadal Mitigation Potential (tCO ₂ e)	HFO	20,700	53,100	489,075	365,625
		MGO	38,150	70,550	506,525	383,075

Source: Author

The highest absolute emission savings (≥ 1.2 million tCO₂e) is demonstrated by Bio-methanol, followed by e-methanol ($\geq 910,000$ tCO₂e). Although grey and blue methanol outperform HFO and MGO, both offer the least savings (max. 95,000 tCO₂e and 176,332 tCO₂e, respectively), underlining their fossil-based origin. These results underscore the critical role of upstream fuel sourcing in determining the lifecycle impacts.

The relative emission reduction shows bio-methanol achieving a net-negative emission profile (~130% reduction) compared to baselines. Following, e-methanol reduces GHG emissions by 96%. Buttressing the emission intensity of their source, grey and blue methanol come last with <20%. These results underpin the stark contrast between pathways, supporting the transformative potentials of carbon-neutral feedstocks and renewables.

For daily avoidance, bio-methanol avoids 195.63–202.61 tCO₂e/day, almost 23 and 13 times that of grey methanol's (8.28–15.26 tCO₂e) avoidance for HFO and MGO. Higher performance is also offered by e-methanol (146.25–153.23 tCO₂e), while blue

methanol (21.24–28.22tCO₂e) is minimal. These results are peculiarly relevant for voyage-level emissions and regulatory compliance (IMO DCS and EU MRV Frameworks).

Bio-methanol provides the optimal decadal mitigation potential (489,075–506,525tCO₂e), followed by e-methanol (365,625–383,075tCO₂e). Grey (20,700–38,150tCO₂e) and blue (53,100–70,550tCO₂e) methanol persist as the least impactful. The long-term climate benefits of low-carbon methanol are fostered by these results.

This environmental analysis affirms that sustainable bio-methanol and e-methanol pathways are effective in maritime decarbonisation. Blue and grey methanol offer no viable solution, as they fall short of net-zero targets. These findings promote renewable methanol production, development of clean-fuel distribution infrastructures, and integration of carbon accounting mechanisms. Furthermore, sustainable methanol is positioned as a cornerstone of maritime decarbonisation strategy due to the magnitude of emission avoidance.

5.2 Techno-Economic Assessment Analysis

This subsection presents and interprets the results of the techno-economic assessment of the integrated system in comparison to conventional propulsion systems. Total Cost of Ownership (TCO), Levelized Cost of Energy (LCOE) and payback periods are assessed under baseline and policy-driven scenarios (using a simplified interpretation of the IMO Framework on Lifecycle GHG Fuel Intensity (2024), and varying carbon price from \$100–\$500). The data (Table 10) for the CAPEX and OPEX calculations were obtained from literature, industry reports, and fuel price comparison websites.

Table 10: CAPEX and Maintenance Values

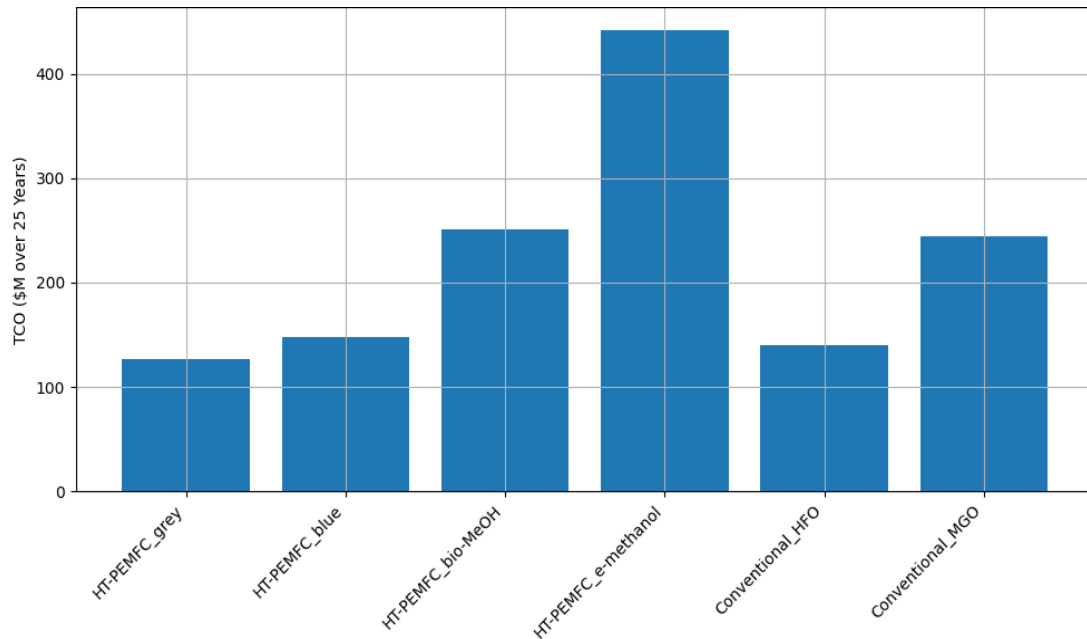
ALTERNATIVES	CAPEX (\$/kW)	OPEX – Yearly Maintenance Cost (\$/kW)	Fuel Costs (\$/tonne)
INTEGRATED METHANOL REFORMER + HT-PEMFC SYSTEM	i. Methanol Reformer = 555.75 ii. PEM Fuel Cells = 854.1 iii. Gearbox = 99.45 iv. Electric Motor = 140.4 v. Methanol Tanks = 0.164 vi. Total = 1,649.46	Calculated as 2% of CAPEX = 32.99	i. Grey Methanol = 350 ii. Blue Methanol = 550 iii. Bio-Methanol = 1198 iv. E-Methanol = 2238
CONVENTIONAL MARINE ENGINES	i. Internal Combustion Engine = 538.55 ii. Fuel Tanks = 0.105 iii. Total = 538.66	Calculated as 2% of CAPEX = 10.77	i. HFO = 442 ii. MGO = 780

Source: (Kanchiralla et al., 2022; Korberg et al., 2021; Methanol Institute, 2024; Ship and Bunker, 2025; Bunker Index, 2025)

5.2.1 Total Cost of Ownership (TCO)

The TCO analysis is insightful for evaluating the long-term economic viability of the propulsion systems (HT-PEMFC and conventional) and fuel sources. It reveals a pronounced cost gradient, highlighting the tensions between economic practicality and decarbonisation significance.

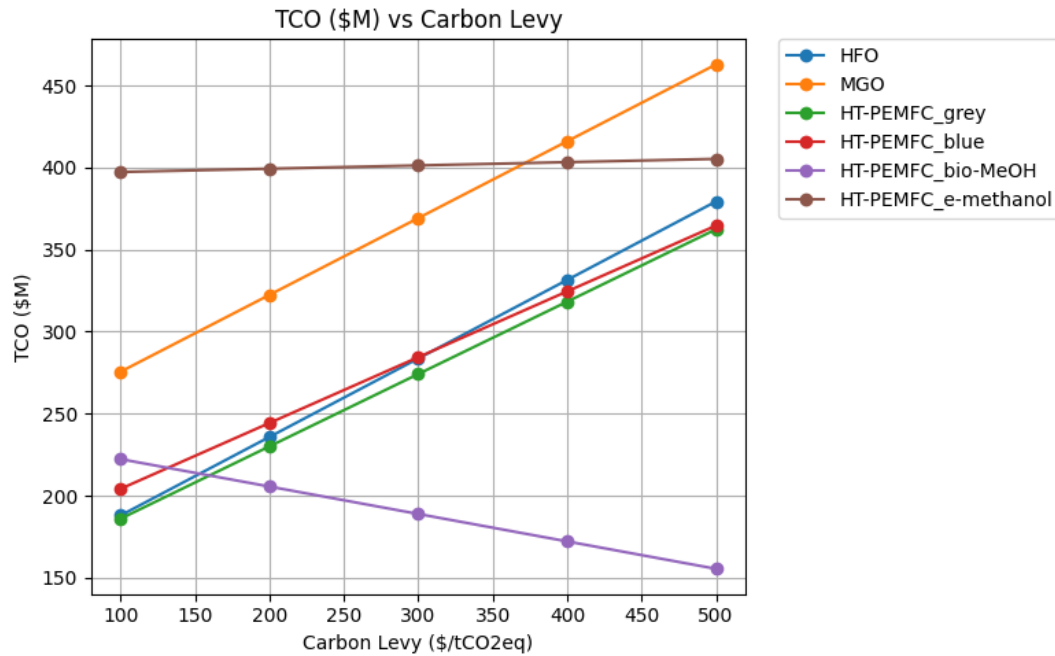
Figure 17 : Baseline TCO



Source: Author

The graph above (Figure 17) shows the baseline TCO. Grey methanol integrated system has the lowest TCO (\$126.7million) among the alternatives, meticulously matched by HFO-powered conventional propulsion system ((\$140million), signifying fuel cost advantage and mature technologies. Blue methanol follows (\$147.8million), reflecting economic carbon capture integration. Comparable high values are presented by bio-methanol (\$250million) and MGO-fuelled (\$246.4million) alternatives. E-methanol emerges as the least favourable (\$440.9million) due to high production cost and immature large-scale synthesis technologies.

Figure 18: Policy-driven TCO



Source: Author

Figure 18 highlights the impact of decarbonisation policies on the TCO of chosen alternatives. There is a substantial TCO increment in conventional alternatives (HFO: \$191.7–\$382.3million, MGO: \$273.7–\$463.4million) and fossil-based methanol pathways (grey: \$185.6–\$359.7million, blue: \$205.1–\$365.6million) due to the inclusion of policy measures. Conversely, bio-methanol (\$221.8–\$158.3million) and e-methanol (\$399–\$408.2million) presented a drop from the baseline value.

Collectively, both scenario analyses highlight a stark contrast between the intrinsic economics of propulsion technologies and their competitiveness under decarbonisation policies. Fossil-based alternatives—HFO, MGO, grey and blue methanol—predominate due to affordability in market-driven scenario, while sustainable options remain underprivileged by high production costs. Fossil-based alternatives are economically attractive, but raises sustainability concerns. However, market-based mechanisms introduced under the policy-driven framework shift the perspectives, internalising environmental externalities to escalate their TCO; while

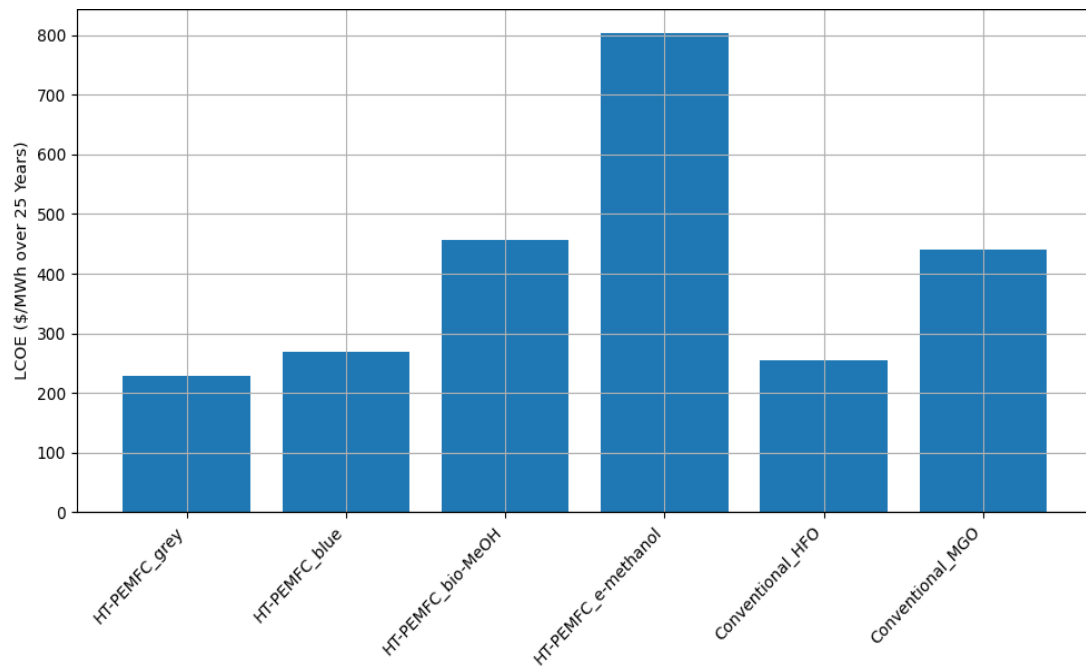
low-emission methanol capitalise on policy incentives, lowering TCO below baseline value.

This polarity emphasises the critical role policy plays in bridging the economic gap between sustainable and carbon-intensive alternatives, demonstrating market force preference for fossil-sourced dominance to the detriment of decarbonisation goals. This analysis supports a phased decarbonisation approach as technologies and policies advance.

5.2.2 Levelized Cost of Energy (LCOE)

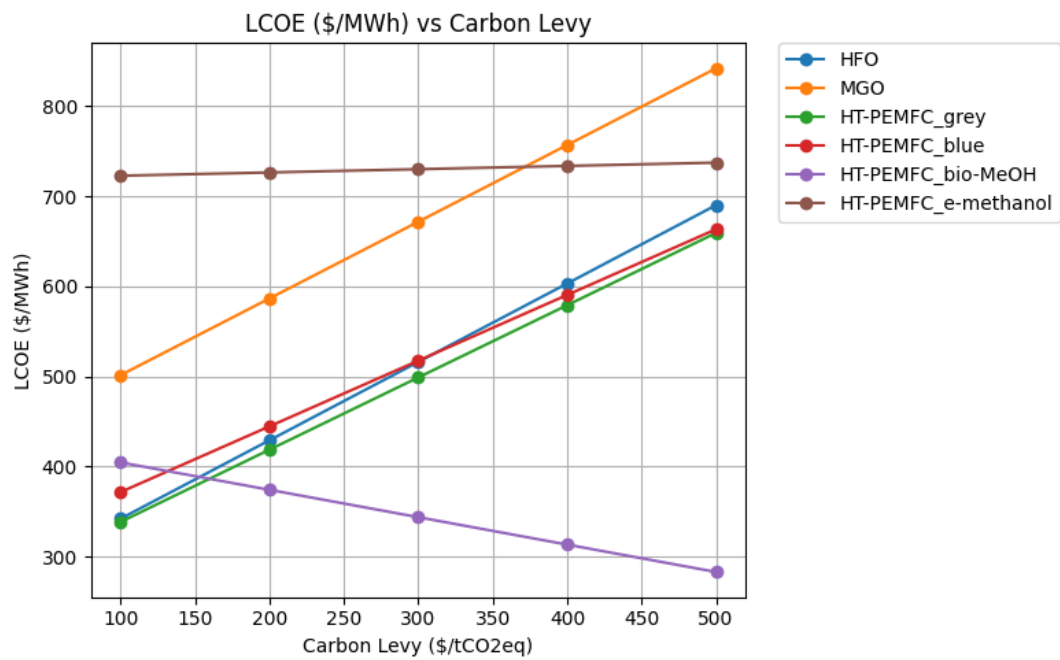
The economic challenges of decarbonisation, underpinning significant disparities over propulsion technologies, are demonstrated by the LCOE analysis. The baseline chart (Figure 19) shows grey-methanol alternative as the most cost-effective, with a \$226/MWh LCOE, followed by HFO-alternative (\$251/MWh) and blue-methanol (\$267/MWh). The limited economies of scale in the current bio-methanol supply chain are reflected in the significantly higher cost (\$457/MWh), nearing MGO (\$440/MWh), which maintains continued competitiveness despite environmental drawbacks. The most expensive (e-methanol at \$804/MWh) signifies high renewable electricity and CO₂ input requirements.

Figure 19: Baseline LCOE



Source: Author

Figure 20: Policy-driven LCOE



Source: Author

Figure 20 shows the policy-driven LCOE of the alternatives, with only bio-methanol (\$407-\$286/MWh) and e-methanol showing reductions (\$726-\$737/MWh) from baseline values, while other methanol alternatives demonstrate higher LCOE (grey: \$337-653/MWh, blue: \$373-\$668/MWh). Similarly, conventional alternatives demonstrated higher LCOE (HFO: \$349-\$692/MWh, MGO: \$501-\$842/MWh).

The disparity between the LCOE charts is mainly due to the introduction of market-based mechanisms, which increase the cost of carbon-positive fuels. In the baseline scenario, LCOE is assessed based on CAPEX and OPEX, but regulations introduced a levy proportional to fuels' WtW emissions. As most lifecycle intensities under review are carbon-positive, the levy increases their effective operative costs and thus, LCOEs. The magnitude of the levy payment sometimes exceeds the benefits from avoided credits or subsidies, yielding higher policy-driven LCOEs than baseline values.

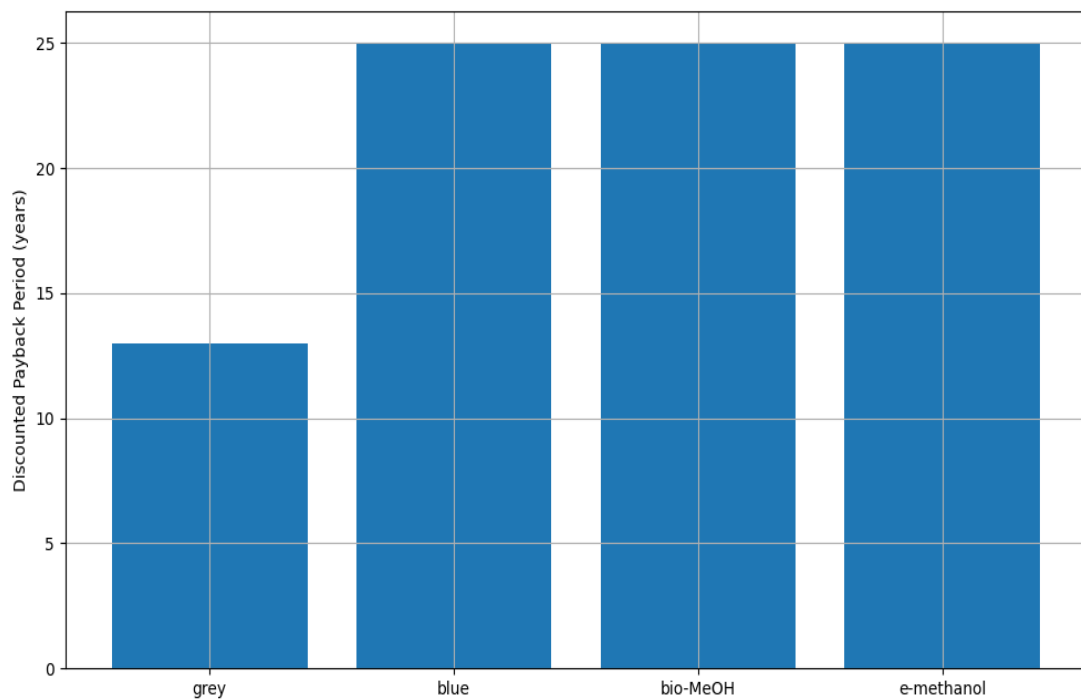
Contrastingly, low carbon-intensity fuels benefit the most, circumventing levies while amassing credits, which lowers LCOE relative to the baseline case. This underscores the intended role of policy, purposefully angling the economic playing field. By rewarding renewable pathways and penalising fossil fuels, the policy incentives mechanisms redefine the market dynamics, ensuring that long-term energy solutions support IMO's decarbonisation target instead of defaulting to fossil-based options.

5.2.3 Payback Period

The payback period analysis shows the relative financial performance and structural barriers hindering their adoption without policy/market incentives. Figure 21 presents the baseline discounted payback period for the methanol-based alternatives, with only the grey-pathway recovering its initial capital expenditure within 13years and the others over 25years (but modelling caps payback limit to lifetime years to enable charts' visualisation), exceeding typical vessel lifespans. This highlights the inherent cost advantage of fossil-based alternatives, and commercial unviability of

decarbonisation-aligned alternatives without policy intervention, amid prevailing market dynamics.

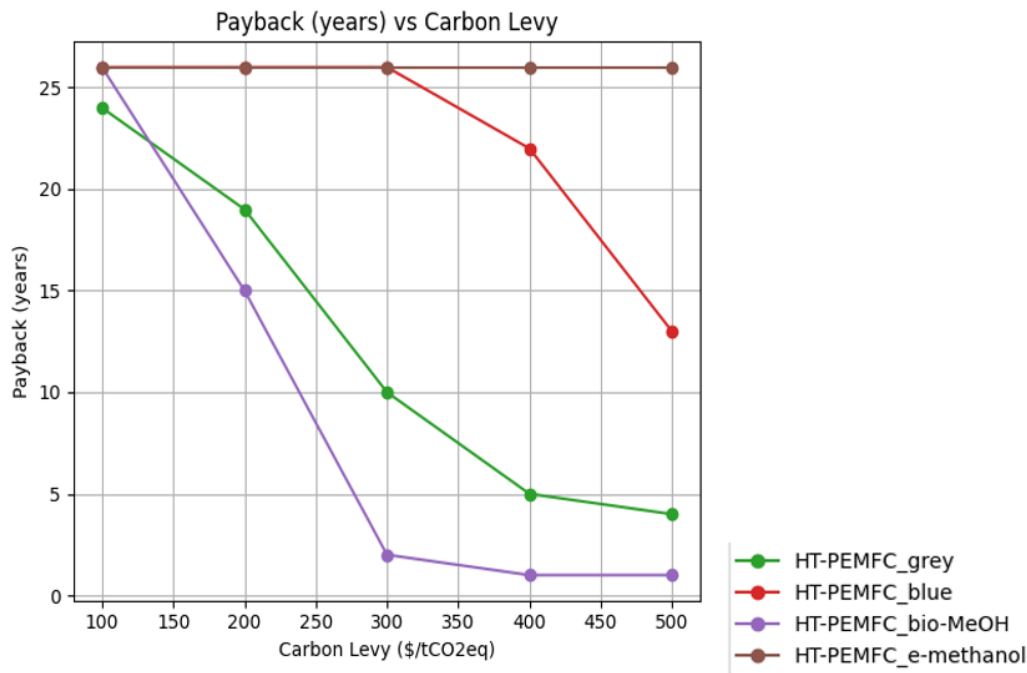
Figure 21: Baseline Payback Period



Source: Author

In the policy-driven (figure 22) scenarios, there is noticeable improvement as all methanol alternatives paid back before the end of vessel's lifetime, while e-methanol remained incapable of paying back within the stipulated time. Despite improving economic performance, policy support benefited fossil-based and negative-emission alternatives.

Figure 22: Policy-Driven Payback Period



Source: Author

The contrast between the scenarios underscores the significant influence of policy in shaping long-term investment parameters. Sustainable alternatives are unattractive with payback periods beyond vessel lifetime, without regulatory or financial intervention. However, policy incentives substantially favour bio-methanol, but e-methanol is profoundly impeded by its high production cost. Although financial policies may improve competitiveness, their efficient design is paramount to prevent the risk of reinforcing dependence on fossil-based alternatives with little contribution to decarbonisation targets. A practical approach to achieve this involves differentiated policy instruments that directly promote financial optimisation for sustainable methanol alternatives or preferential financing to narrow the gap with fossil and transitional alternatives.

These results underpin the systemic interrelationship between institutional frameworks and technological maturity. The uptake of the integrated system may be

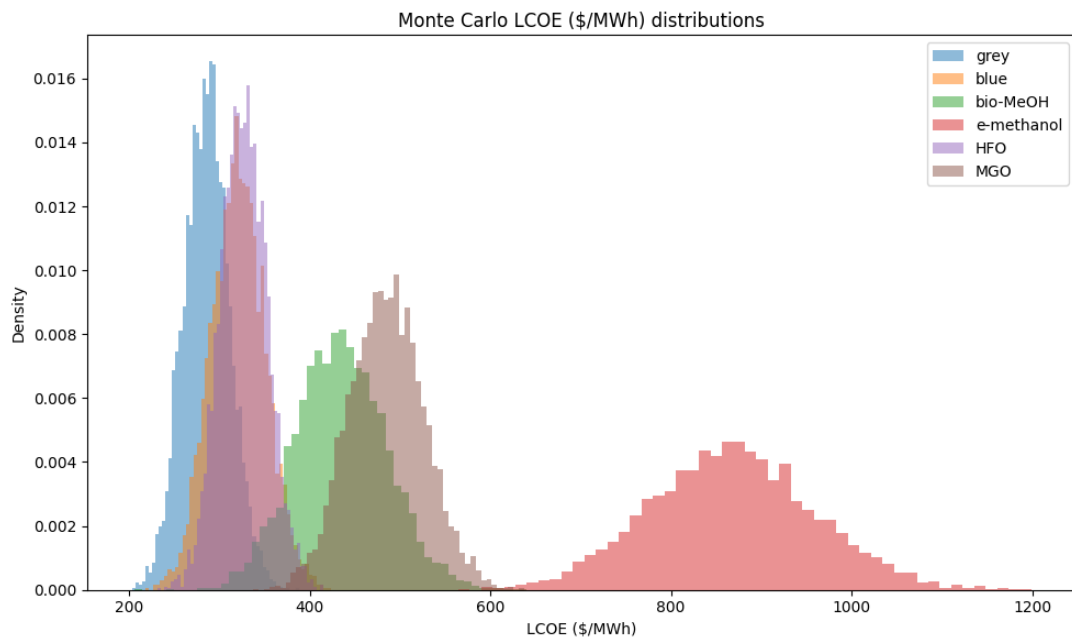
technologically viable, but constrained by economic feasibility, necessitating critical external intervention, i.e., regulatory frameworks. This confirms that maritime decarbonisation is not solely technologically-dependent, but necessitates an integrated framework—regulations, financial innovations and market-based incentives—to realign private investment decisions to the global decarbonisation path.

5.2.4 Uncertainty Simulation Analysis

Monte Carlo simulations (based on 10,000 iterations) present distinctive risk profiles for the propulsion alternatives. Parameters incorporated are CAPEX ($\pm 10\%$), fuel prices ($\pm 10\%$), and propulsion efficiencies ($\pm 5\%$).

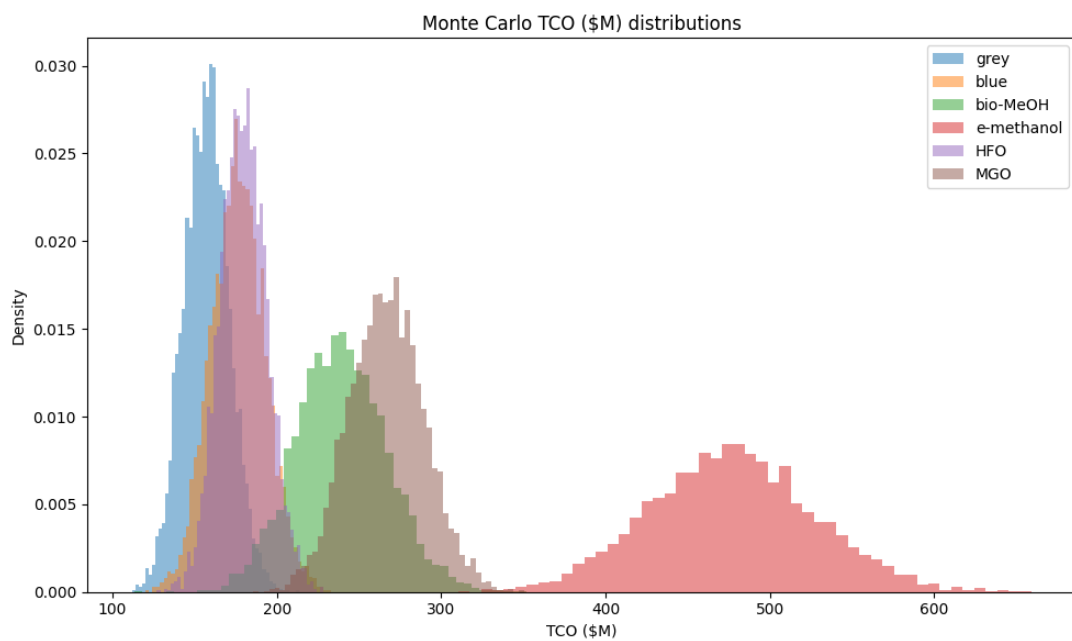
The LCOE distribution (Figure 23) shows grey-methanol and HFO-conventional alternatives distributions fluctuating between 200-350\$/MWh with low variance, denoting robust cost competitiveness under volatility, while blue-methanol illustrates moderate spreads implying sensitivity to price changes. MGO-conventional behaves similarly to bio-methanol (380-550\$/MWh) whose competitiveness is over-reliant on policies. E-methanol shows higher variance (630-1150\$/MWh), caused by cost uncertainties of fuel production.

Figure 23: Sensitivity LCOE Distribution



Source: Author

Figure 24: Sensitivity TCO Distribution



Source: Author

The TCO (figure 24) reiterates LCOE patterns. All alternatives, except e-methanol, have clustered distribution around \$100-300million over vessel's lifetime, indicating low-risk investments. Habitually, e-methanol (\$400-600million) indicates an immoderate risk zone, emphasising scaling-up challenges.

These Monte Carlo distributions reiterate the inherent uncertainties in maritime propulsion economics. Although fossil fuels offer lower risks and faster paybacks, sustainable options will gain economic viability under strong policy interventions, supporting net-zero alignment.

CHAPTER 6

6.1 Conclusion

This dissertation evaluated the feasibility of integrating methanol steam reforming with high-temperature proton exchange membrane fuel cells for seagoing vessel propulsion, presenting a holistic analysis covering technical, economic and environmental aspects. The findings confirm the technical and environmental superiority of the system to conventional propulsion systems; however, real-world viability transcends performance metrics.

Environmentally, the lifecycle analysis confirms a significant reduction in well-to-wake GHG emissions by bio-methanol and e-methanol pathways, positioning them as a cornerstone for achieving global net-zero ambitions. However, these benefits are moderated by economic constraints, including capital intensity and vulnerability to market volatility. In contrast, fossil-derived grey and blue methanol pathways perform similarly to conventional fuels, with substantial environmental constraints.

The study also highlighted the operational promise and complexity of the integrated system. The integration offers modularity and synergy with the thermal management system, improving energy efficiency and vessel resilience, yet is associated with challenges. Methanol's lower energy density requires roughly double the storage space in comparison to conventional fuels, and the integrated system superimposes thermal and control requirements, escalating their complexity. These constraints underscore the feasibility of the integrated system beyond laboratory efficiencies to extensive shipboard operational aspects such as power and thermal management and redundancy.

Economically, the techno-economic assessment emphasises the importance of policy intervention, as fossil-based methanol pathways and conventional fuels dominate under market-driven conditions, owing to lower fuel costs and mature technologies.

However, regulatory incentives (market-based mechanisms) substantially increase the cost of carbon-positive fuels in the policy-driven scenarios (which ranged carbon levy from \$100–\$500), shifting competitiveness towards sustainable options. Bio-methanol was especially advantaged by regulatory support, while e-methanol was marginally impeded by high production cost, although performing better than fossil-based fuels. These findings are supported by Monte Carlo simulations, which showed fossil and transitional fuels clustered in a low-risk zone while sustainable options face higher volatility.

In summary, the feasibility of this propulsion technology depends on critical enablers, including tactical infrastructure investment in sustainable methanol supply chain and bunkering network, technological maturity to overcome operational barriers, and internalisation of carbon externalities while incentivising sustainable methanol with policy frameworks. Therefore, addressing these technical and institutional challenges requires orchestrated collaboration between policymakers, industry players and researchers. This study contributes a comprehensive framework that synthesises technical progress with policy imperatives and market dynamics—supporting decarbonisation technologies for maritime propulsion.

6.2 Recommendations

1. Regulators and policymakers should implement differentiated market-based mechanisms to penalise fossil-based fuels, and a predictable and transparent subsidy framework to reduce investor uncertainty, thus de-escalating early-investment risks. Safety and certification standards for methanol handling and onboard reforming should be harmonised across the IMO, EU and classification societies to ensure scalable and innovative deployment of methanol technologies.
2. Research institutions and fuel cell developers should focus on improving modular designs to ensure scalable power and redundancy for larger vessels.

3. The shipbuilding industry is recommended to design ship layout for storage optimisation without compromising cargo capacity, while shipbuilders should integrate an advanced Energy Management System to optimise thermal and electrical distribution.
4. Financing bodies, port authorities and infrastructure planners are recommended to foster incentives to align technology and fuel production, availability and distribution; by expanding sustainable production capacity and bunkering infrastructure across major shipping hubs.

6.3 Further Research

Considering the scope and limitations of this study, further studies are recommended as follows to promote this propulsion technology under review:

1. Dynamic modelling of the integrated system under transient maritime operating conditions (start-up/shut-down periods, load changes and emergency scenarios) for seagoing vessels. Furthermore, its life-extension strategies in comparison to conventional marine engines should be examined.
2. The techno-economic assessment should be expanded to incorporate the detailed analysis of the IMO Net-Zero Framework and quantify the impact of subsidy structures (fixed, performance-based and sliding-scale) on sustainable methanol competitiveness.
3. Finally, lifecycle assessment should include socio-technical and socio-environmental impacts of methanol feedstocks and the integrated system.

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Appendices

Appendix 1: Comparison of Fuel Cell Types

Fuel Cell Type	LT-PEM HT-PEM	SOFC	MCFC	PAFC	AFC	DMCF
Fuel Options	Hydrogen	Hydrocarbons, Hydrogen, Methanol	Hydrocarbons, Hydrogen, Methanol	NG/LNG, Hydrogen, Methanol	Hydrogen	Methanol
Electrolyte	Water-based polymer membrane Mineral-acid based polymer membrane	Porous ceramic material (Yttria-stabilised Zirconium)	Molten carbonate salt	Phosphoric Acid	Potassium Hydroxide	Water-based polymer membrane
Anode Cathode	Platinum Platinum	Nickel Alloy Lithium Strontium Manganite	Nickel Alloy Nickel-Oxide Lithium	Platinum-Carbon Platinum-Carbon	Nickel Silver	Platinum-Ruthenium Platinum-Ruthenium
Operating Temperature (°C)	50-110 160-220	500-1000	600-700	150-220	50-230	75-120
Electrical Efficiency	45%-60% (80% Overall for HT-PEMFC)	50%-60% (85% Overall)	50%-60% (85% Overall)	45%-55% (80% Overall)	40%-55%	20%-30%
Emission	H ₂ O	H ₂ O + CO ₂ if carbon-based fuel is used	H ₂ O + CO ₂ if carbon-based fuel is used	H ₂ O + CO ₂ if carbon-based fuel is used	H ₂ O	H ₂ O + CO ₂
Power Output	≤1MW (up to 200Kw per module)	≤1MW (up to 250Kw per module)	≤1MW (up to 250Kw per module)	≤1MW (100Kw-400kW per module)	≤500kW (up to 100Kw per module)	≤7kW (up to 2kW per module)
Size	Small	Medium	Large	Large	Small	Small
Power Density(W/cm ²)	0.3-0.8	0.1-0.3	0.1-0.2	0.1-0.3	0.05-0.2	0.15-0.3
Relative Cost	Low Medium	High	High	Medium	Low	Medium
Lifetime (hours)	60000-80000 40000 (transport)	20000-40000	15000-30000	40000-60000	5000-8000	10000-20000
Drawbacks	CO + S poisoning	S poisoning, cycling effects, mechanically fragile, long start-up time	S poisoning, cycling effects, long start-up time	CO + S poisoning	CO ₂ poisoning	Methanol crossover
Waste Heat Recovery	N/A Heat Exchanger/Steam Turbine	Heat Exchanger/Steam Turbine/Gas Turbine	Heat Exchanger/Steam Turbine/Gas Turbine	Heat Exchanger/Steam Turbine	N/A	N/A
Application	Backup power, Portable power, Distributed	Auxiliary power, Electric utility, Distributed Generation, Transportation	Electric utility, Distributed generation	Distributed generation	Military, Space, Backup power, Transportation	Portable power, Material-handling Vehicles, Backup power and UPS

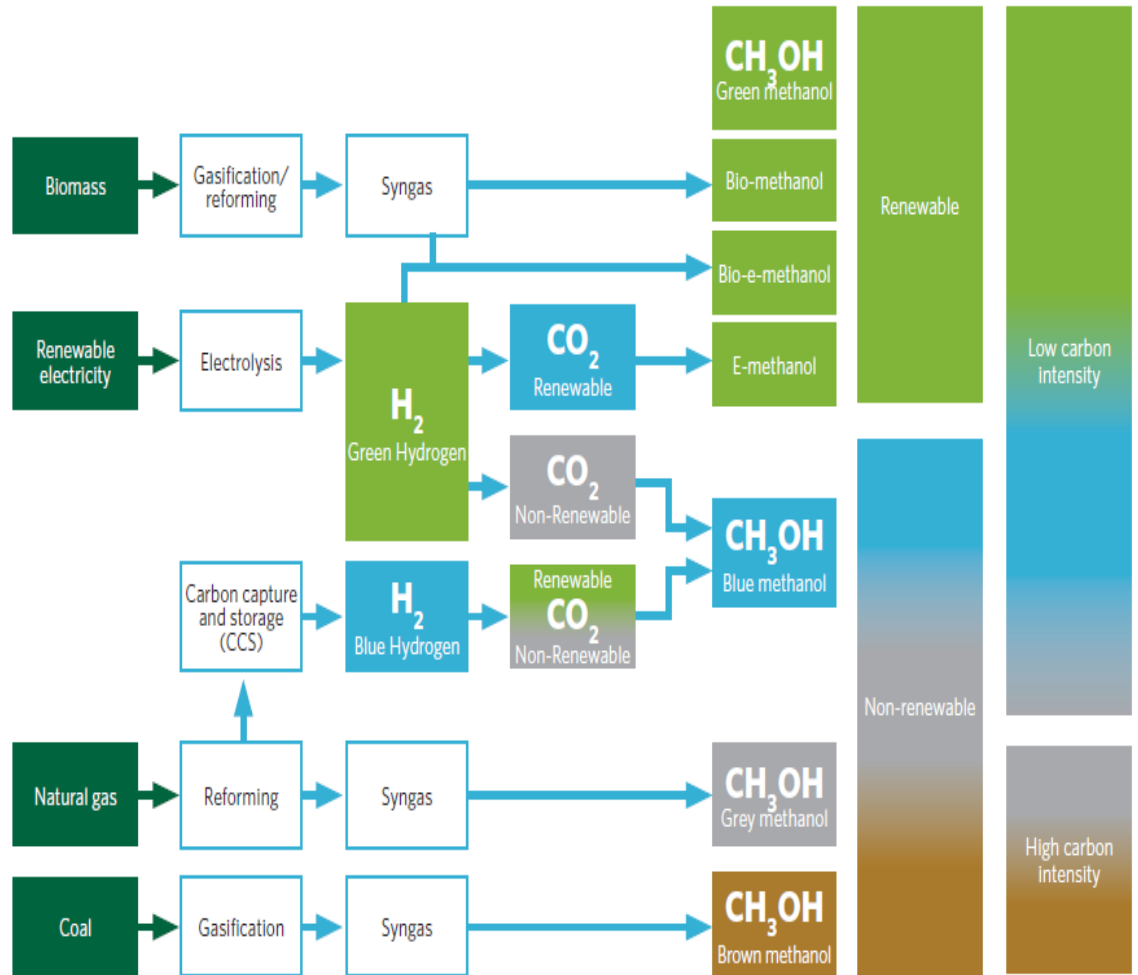
Source: Author

Appendix 2: Comparative Fuels Properties

	Diesel	Methanol	Ethanol	LNG	Hydrogen
Density (kg m^{-3})	833–881	798	794	450	0.0838
Auto-ignition temperature (K at 1 bar)	530	743	635	810	858
Flammability limits (vol. % air)	0.7–5	6–36	3–19	4–16	4–75
Stoich. air–fuel ratio on mass basis	14.5	6.5	9.1	17.2	34.3
Net heating value (MJ/kg)	42.5	20.1	27.0	46–50.2	119.9
Flame velocity (cm/s)	30	50	41	380	265–325
Flame temperature (K at 1 bar)	2327	2163	2193	2233	2318
Octane number	30	109	109	120	130
Cetane number	40–55	<5	8	–10	–
Fuel carbon content (wt %)	85	38	52	75	0
Fuel hydrogen content (wt %)	15	12	13	25	100
Fuel oxygen content (wt %)	0	50	35	0	0
Fuel sulfur content (wt %)	<350 ppm	0	0	0	0

Source: Deniz and Zincir, 2016

Appendix 3: Illustration of Methanol Production Pathways



Source: The Methanol Institute (2023)

Appendix 4: Modelling Parameters and Operating Conditions

Parameter	Description	Value	Unit
METHANOL STEAM REFORMER SUBSYSTEM			
R	Ideal Gas Constant		J/K.mol
T_0	Reformer Inlet Temperature	523.15	K
T_{ref}	Reference temperature	298.15	K
LHV_{H_2}	Lower Heating value of Hydrogen	240×10^3	J/mol
LHV_{CH_3OH}	Lower Heating value of Methanol	638×10^3	J/mol
$\Delta H_{vap,CH_3OH}$	Latent Heat of Vaporization (Methanol)	38×10^3	J/K.mol
$\Delta H_{vap,H_2O}$	Latent Heat of Vaporization (Hydrogen)	40.7×10^3	J/K.mol
C_{p,CH_3OH}	Heat Capacity (Methanol) at 523K	44.1	J/K.mol
C_{p,H_2O}	Heat Capacity (Water Vapour/Steam) at 523K	33.6	J/K.mol
$C_{p,gas}$	Average Gas Heat Capacity	29.1	J/K.mol
$C_{p,cat}$	Catalyst Heat Capacity	1000	J/K.kg
ρ_{cat}	Catalyst Bulk Density	2000	Kg/m ³
ΔH_1	Reaction Enthalpy (MSR)	49.5	kJ/mol
ΔH_2	Reaction Enthalpy (MD)	90	kJ/mol
ΔH_3	Reaction Enthalpy (WGS)	-41	kJ/mol
k_1	Pre-exponential factor (MSR)	1×10^4	mol/kg.s
k_2	Pre-exponential factor (MD)	1×10^5	mol/kg.s
k_3	Pre-exponential factor (WGS)	5×10^3	mol/kg.s
E_{a_1}	Reaction Activation Energy (MSR)	90×10^3	J/mol
E_{a_2}	Reaction Activation Energy (MD)	100×10^3	J/mol
E_{a_3}	Reaction Activation Energy (WGS)	80×10^3	J/mol
L	Length of [Methanol Steam] Reformer	2	m
u	Superficial Gas Velocity	0.005	m/s
P_{total}	Total Reactor Pressure		
U_{loss}	Heat Loss Coefficient	120	W/m ³ .K
A_m	Area of membrane per reactor length	0.3	m ² /m

$P_{H_2,perm}$	Hydrogen Permeability Constant	8000	mol/m ² .s.Pa ^{-0.5}
p_{perm}	Hydrogen pressure on the permeate side	9000	Pa
α	Gas-solid Heat Capacity Weighting factor	0.2	
HT-PEM FUEL CELL SUBSYSTEM			
F	Faraday's Constant	96485	C/mol
T_{fc}	Operating temperature	433.15	K
n_{cell}	Number of cells in a stack	455	
A_{cell}	Active Area per cell	0.17	m ²
P_{O_2}	Oxygen Partial Pressure (air)	0.21	Atm
P_{H_2O}	Water Vapour Partial Pressure	0.1	Atm
E_0	Open-Circuit Voltage	1.05	V
j_0	Exchange Current Density	1.2×10^{-3}	A/cm ²
j_{lim}	Limiting Current Density	1.3	A/cm ²
j	Current Density Sweep	0 - 0.3	A/cm ²
R_{ohmic}	Ohmic Resistance	0.1	Ωcm^2
P_{Total}	Total Pressure	1	Atm
α_a	Anodic Transfer Coefficient	0.5	
α_c	Cathodic Transfer Coefficient	0.5	

Source: Li et al, 2023; Zhuang et al., 2023; and Zhu et al., 2019.

Appendix 5: Summary of Reformer Parameters Trends with Varying Inlet Temperature

Parameter	493K	513K	533K	553K	Temperature Trend
Methanol conversion	Low	Moderate	High	Very High	Elevates due to enhanced reaction kinetics reactions
Hydrogen yield	Moderate	High	Higher	Highest	Increases as the temperature favours H ₂ formation
CO molar fraction	Low	Rising	Peak	Declines	Increases slightly (493–533K) but reduces at 553K due to increased WGS reaction
CO ₂ molar fraction	Moderate	High	High	Highest	Even increase because of MSR and WGS reactions
Reaction rate	Slow	Moderate	Faster	Fastest	Accelerates with temperature
Catalyst activity	Suboptimal	Improving	Optimal	Highly active	Improves with increasing temperature
Selectivity to hydrogen	Moderate	Higher	High	Highest	Enhanced at elevated temperatures

Appendix 6: Materials Quantities for Design of System

Meticulous estimation of material quantities for the design and simulation of the integrated MSR + HT–PEMFC system is consequential to ensure feasibility, performance alignment with modelled parameters and cost–effectiveness. The modelled system simulates a MSR for hydrogen production at 1.4mol/s for a 160kW HT–PEMFC stacks under full load (comprising 455cells, each having an active area of 0.17m² totalling **77.35m²**). Estimated material quantities estimates (prototypical thickness, loadings, densities and scaling) are based on standard engineering assumptions derived from literature and manufacturer's datasheets, including 10–20% margins for assembly tolerances, fabrication losses and operational viability to ensure manufacturing sufficiency. Assumptions such as PBI membrane thickness (80–100µm) and catalyst loadings (0.5–1.0mg/cm²) are drawn from established values in fuel cell engineering and scaled to the code stack's specification. Membrane area (4.2m² for Pd–Ag) is assumed for the MSR to align with reactor length and hydrogen permeation flux in the code.

Table A : Estimated Quantities for Production of the Integrated MSR + HT–PEMFC System

Subsystem	Material	Component	Estimated Quantity	Assumptions/Rationale
HT–PEMFC	Polybenzimidazole (PBI)		10.61kg	Typical thickness per membrane = 100µm, density = 1.3g/cm ³ (1300kg/m ³), volume = total active area x thickness = 77.35m ² x 0.0001 = 0.0077m ³ ; mass = volume x density = 0.0077 x 1300 = 10.01kg + 2%

	Platinum alloy	Catalyst layer (CL)	0.65kg	Combined typical loading ² = 0.8mg/cm ² , mass = total active area (in cm ²) x loading = (0.8 x 773500)/1000 = 619g + 5%
	Carbon cloth (with PTFE)	Gas Diffusion Layer (GDL)	19kg	Typical areal weight = 120g/m ² , thickness = 350µm (2 GDLs/cell), mass/cell = areal weight x active cell area = 2 x 120 x 0.17 = 41g, stack mass = Mass _{cell} x n _{cell} = (41 x 455) /1000 = 18.66kg + 2%
	Graphite composites	Bipolar plates	232kg	Typical thickness = 1.5mm, density = 1.85g/cm ³ , area per plate ≈ 0.18m ² , mass/cell = area x thickness x density = 0.18 x 0.0015 x 1850 = 0.5kg. Mass _{stack} = mass/cell x n _{cell} = 0.5 x 455 = 227.5kg + 2%
	Graphite composites	Seals/gaskets	2.32kg	Typical weight per cell ≈ 5g, Weight for stack = weight/cell x n _{cell} = (5 x 455)/ 1000 = 2.275kg + 2%

²Value used is combined loading of anode and cathode, which is higher in HT-PEMFC than LT-PEMFC for reformate tolerance.

	Stainless alloy	Stack end plates ³	84kg	Thickness _{/plate} ⁴ $\approx$ 20–30mm, area $\approx$ 0.2m ² , density ⁵ = 8g/cm ³ , mass _{/plate} = thickness _{/plate} x area x density = 0.025 x 0.2 x 8000 = 40kg x 2 = 80kg + 5%
--	-----------------	-------------------------------	------	---

Source: Author

1. Transportation: Shipping of materials from Japan to Aarhus port (Denmark) has distance of 15,368n.miles, and from Aarhus port to shipyard (Dalian, China) (~14,116n.miles) and road transport from Aarhus port to BlueWorld Technologies, Aalborg and vice-versa (~352km x 2).

³ There are typically 2 end plates for a stack.

⁴ The mean of the range was used for calculation (25mm)

⁵ Approximate density for 316L Grade Stainless Steel

Appendix 7: Recycling Credit for HT-PEMFC Materials

S/N	Material	Emission factors (WtT) (kgCO ₂ e/kg)	Recycling Rate (%)	Material Quantity	Recycling Credit (kgCO ₂ e)
1.	Polybenzimidazole (PEM)	8.87	87	10.61	81.88
2.	Platinum (catalyst layer)	33400	95	0.65	20624
3.	Carbon cloth (gas diffusion layer)	N/A	-	19	-
4.	Graphite composites (bipolar plates)	5.34	87	232	1077.83
5.	Graphite composites (seals/gaskets)	5.34	87	2.32	10.78
6.	Stainless alloy (end plates)	5.13	87	84	374.9
Total Recycling Credit					22169.88

Source: Author

Appendix 8: Modelling Code of Integrated Reformed Methanol HT-PEMFC System

```
import numpy as np
from scipy.integrate import solve_ivp, simpson
import matplotlib.pyplot as plt
import pandas as pd
from scipy.integrate import simpson
from scipy.optimize import root_scalar
# Constants
R = 8.314 # J/mol/K
T0 = 523.15 # K (initial temperature, 250°C)
P_total = 101325 # Pa
LHV_H2 = 240e3 # J/mol (lower heating value of H2)
LHV_CH3OH = 638e3 # J/mol (lower heating value of CH3OH)
Cp_CH3OH = 44.1 # J/mol/K (methanol gas heat capacity at ~523 K)
Cp_H2O = 33.6 # J/mol/K (water vapor heat capacity at ~523 K)
T_ref = 298.15 # K (reference temperature for sensible heat)
deltaH_vap_CH3OH = 38e3 # J/mol (latent heat of vaporization for methanol)
deltaH_vap_H2O = 40.7e3 # J/mol (latent heat of vaporization for water)
U_loss = 120 # W/m³ (heat loss coefficient)
process_eff = 0.85 # Process efficiency factor
# Reactor and catalyst parameters
length = 2.0 # m
A_membrane = 0.3 # m²/m reactor length
P_H2_perm = 8000 # mol/(m²·s·Pa0.5)
p_perm = 9000 # Pa (permeate side H2 pressure)
u = 0.005 # m/s (superficial velocity)
rho_cat = 2000 # kg/m³ catalyst bulk density
Cp_gas = 29.1 # J/mol/K (average gas heat capacity)
Cp_cat = 1000 # J/kg/K (typical solid catalyst heat capacity)
alpha = 0.2 # gas/catalyst heat capacity weighting factor
```

```

# Heats of reaction (J/mol, ordered as SRM, Methanol Decomposition, WGS)
deltaH1 = 49.5e3 # CH3OH + H2O → CO2 + 3H2 (SRM, endothermic)
deltaH2 = 90e3 # CH3OH → CO + 2H2 (MD, endothermic)
deltaH3 = -41e3 # CO + H2O → CO2 + H2 (WGS, exothermic)
# Initial concentrations (mol/m³)
C_CH3OH0 = 2500
C_H2O0 = 3750
C_CO0 = 0
C_CO2_0 = 0
C_H2_0 = 0
# Kinetic parameters
k1_0 = 1.0e4 # SRM, mol/(kg_cat·s)
Ea1 = 90e3
k2_0 = 1.0e5 # CH3OH decomposition, mol/(kg_cat·s)
Ea2 = 100e3
k3_0 = 5.0e3 # WGS, mol/(kg_cat·s)
Ea3 = 80e3
def rate_constants(T):
    k1 = k1_0 * np.exp(-Ea1 / (R * T))
    k2 = k2_0 * np.exp(-Ea2 / (R * T))
    k3 = k3_0 * np.exp(-Ea3 / (R * T))
    return k1, k2, k3
def reactor_model(z, y):
    C_CH3OH, C_H2O, C_CO, C_CO2, C_H2, T, H2_perm_cum = y
    k1, k2, k3 = rate_constants(T)
    # Ensure non-negative concentrations
    C_CH3OH = max(C_CH3OH, 0)
    C_H2O = max(C_H2O, 0)
    C_CO = max(C_CO, 0)

```

```

C_CO2 = max(C_CO2, 0)
C_H2 = max(C_H2, 0)
# Reaction rates
r1 = k1 * C_CH3OH * C_H2O # CH3OH + H2O → CO2 + 3H2 (SRM)
r2 = k2 * C_CH3OH # CH3OH → CO + 2H2 (decomposition)
r3 = k3 * C_CO * C_H2O # CO + H2O → CO2 + H2 (WGS)
# Hydrogen permeation flux
J_H2 = P_H2_perm * (np.sqrt(max(C_H2 * R * T, 0)) - np.sqrt(p_perm))
J_H2 = max(J_H2, 0) # Ensure non-negative flux
# Mass balances
dCH3OH_dz = (-r1 - r2) / u
dH2O_dz = (-r1 - r3) / u
dCO_dz = (r2 - r3) / u
dCO2_dz = (r1 + r3) / u
dH2_dz = (3*r1 + 2*r2 + r3 - J_H2 * A_membrane) / u
dH2_perm_cum_dz = J_H2 * A_membrane / u
# Energy balance (non-isothermal)
Q_rxn = r1 * deltaH1 + r2 * deltaH2 + r3 * deltaH3 # W/m³
Q_loss = U_loss * (T - T_ref) # Heat loss to surroundings
total_Cp = alpha * Cp_gas * sum([C_CH3OH, C_H2O, C_CO, C_CO2, C_H2]) +
(1 - alpha) * rho_cat * Cp_cat
dT_dz = -(Q_rxn + Q_loss) / (u * total_Cp)

return [dCH3OH_dz, dH2O_dz, dCO_dz, dCO2_dz, dH2_dz, dT_dz,
dH2_perm_cum_dz]
# Initial conditions and reactor domain
y0 = [C_CH3OH0, C_H2O0, C_CO0, C_CO2_0, C_H2_0, T0, 0.0]
z_span = (0, length)
z_eval = np.linspace(0, length, 200)
# Solve ODEs

```

```

sol = solve_ivp(reactor_model, z_span, y0, t_eval=z_eval, method='BDF', rtol=1e-6,
atol=1e-8)
z = sol.t
C_CH3OH, C_H2O, C_CO, C_CO2, C_H2, T_profile, H2_perm_cum = sol.y

# Permeate H2 profile
H2_perm_profile = np.gradient(H2_perm_cum, z)
# Define total hydrogen (retentate + permeate)
H2_total = C_H2 + H2_perm_cum
# Energy calculations
methanol_consumed = C_CH3OH0 - C_CH3OH[-1]
water_consumed = C_H2O0 - C_H2O[-1]
energy_input_methanol = methanol_consumed * LHV_CH3OH
energy_sensible_CH3OH = methanol_consumed * Cp_CH3OH * (T0 - T_ref)
energy_sensible_H2O = water_consumed * Cp_H2O * (T0 - T_ref)
energy_latent_CH3OH = methanol_consumed * deltaH_vap_CH3OH
energy_latent_H2O = water_consumed * deltaH_vap_H2O
def reaction_heat_endothermic(z, y):
    C_CH3OH, C_H2O, C_CO, C_CO2, C_H2, T, _ = y
    k1, k2, _ = rate_constants(T)
    r1 = k1 * C_CH3OH * C_H2O
    r2 = k2 * C_CH3OH
    return r1 * deltaH1 + r2 * deltaH2
def heat_loss(z, y):
    T = y[5]
    return U_loss * (T - T_ref)
Q_rxn_endothermic = np.array([reaction_heat_endothermic(z[i], sol.y[:, i]) for i in
range(len(z))])
Q_loss_profile = np.array([heat_loss(z[i], sol.y[:, i]) for i in range(len(z))])
net_reaction_heat = simpson(Q_rxn_endothermic, z)

```

```

heat_losses = simpson(Q_loss_profile, z)
energy_input = (energy_input_methanol +
                energy_sensible_CH3OH +
                energy_sensible_H2O +
                energy_latent_CH3OH +
                energy_latent_H2O +
                max(net_reaction_heat, 0) +
                heat_losses)

energy_output = H2_perm_cum[-1] * LHV_H2 * process_eff
system_efficiency = (energy_output / energy_input) * 100 if energy_input > 0 else 0

# Performance metrics

# Hydrogen yield calculation
H2_retentate_total = simpson(y=C_H2, x=z)
H2_permeated_total = simpson(y=H2_perm_profile, x=z)
H2_total_mol = H2_retentate_total + H2_permeated_total # mol/m²
CH3OH_reacted_mol = methanol_consumed * length # mol/m²
H2_yield = H2_total_mol / (3 * CH3OH_reacted_mol) * 100 if CH3OH_reacted_mol
> 0 else 0

# Other metrics
CH3OH_conversion = methanol_consumed / C_CH3OH0 * 100
permeate_H2_purity = 100.0 # assuming perfect membrane selectivity
retentate_H2_purity = C_H2[-1] / (C_H2[-1] + C_CO2[-1] + C_CO[-1]) * 100 if
(C_H2[-1] + C_CO2[-1] + C_CO[-1]) > 0 else 0
final_CO_retentate = C_CO[-1]

# -----
# Extract PH2_out for Fuel Cell
# -----

C_total_exit = C_CH3OH[-1] + C_H2O[-1] + C_CO[-1] + C_CO2[-1] + C_H2[-1]
y_H2 = C_H2[-1] / C_total_exit if C_total_exit > 0 else 0
PH2_out = y_H2 * (P_total / 101325) # atm

```

```

# Display results
print(f"Hydrogen Yield: {H2_yield:.2f}%")
print(f"Methanol Conversion: {CH3OH_conversion:.2f}%")
print(f"Final CO concentration (Retentate Side): {final_CO_retentate:.6f} mol/m3")
print(f"MSR System Efficiency: {system_efficiency:.2f}%")

# -----
# HT-PEMFC Stack Model
# -----

F = 96485 # C/mol
T_fc = 433.15 # K
n_cells = 455
A_cell = 0.17 # m2
A_cell_cm2 = A_cell * 1e4
PO2 = 0.21 # atm
P_H2O = 0.1 # atm

# Nernst open-circuit voltage
E0 = 1.05 # V
E_nernst = E0 - (R * T_fc / (2 * F)) * np.log((PH2_out * PO2**0.5) / P_H2O)

# Electrochemical parameters
j0 = 1.2e-3 # A/cm2
R_ohmic = 0.1 # ohm·cm2
j_lim = 1.3 # A/cm2
alpha_a = 0.5
alpha_c = 0.5
n_e = 2
j_range = np.linspace(0, 0.3, 100)
V_cell, I_stack, P_stack, efficiency = [], [], [], []
def solve_eta_act(j, T_fc, j0, alpha_a, alpha_c):
    def bv_eq(eta):
        term1 = np.exp((alpha_a * F * eta) / (R * T_fc))

```

```

    term2 = np.exp(-(alpha_c * F * eta) / (R * T_fc))
    return j - j0 * (term1 - term2)

result = root_scalar(bv_eq, bracket=[-1, 1], method='brentq')
return result.root if result.converged else np.nan

for j in j_range:
    eta_act = solve_eta_act(j, T_fc, j0, alpha_a, alpha_c)
    eta_ohmic = j * R_ohmic
    eta_conc = -(R * T_fc / (n_e * F)) * np.log(1 - j / j_lim) if j < j_lim else np.inf
    V = E_nernst - eta_act - eta_ohmic - eta_conc
    I_total = j * A_cell_cm2
    P_total = I_total * V * n_cells / 1000 # kW
    H2_mol_rate = (I_total * n_cells) / (2 * F)
    P_H2 = H2_mol_rate * 241.8e3 / 1000 # LHV in kJ/mol
    eta = P_total / P_H2 if P_H2 > 0 else 0
    V_cell.append(V)
    I_stack.append(I_total)
    P_stack.append(P_total)
    efficiency.append(eta)

V_cell = np.array(V_cell)
I_stack = np.array(I_stack)
P_stack = np.array(P_stack)
efficiency = np.array(efficiency)

# -----
# Plotting
# -----

plt.figure(figsize=(8, 5))
plt.plot(I_stack, V_cell * n_cells, label='Stack Voltage (V)')
plt.xlabel('Stack Current (A)')
plt.ylabel('Voltage (V)')
plt.title('HT-PEMFC Stack Voltage vs Current')

```

```

plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()
plt.figure(figsize=(8, 5))
plt.plot(I_stack, P_stack, color='green', label='Stack Power (kW)')
plt.xlabel('Stack Current (A)')
plt.ylabel('Power Output (kW)')
ong
plt.title('HT-PEMFC Stack Power vs Current')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()
plt.figure(figsize=(8, 5))
plt.plot(I_stack, efficiency * 100, label='Stack Efficiency (%)', color='red')
plt.xlabel('Stack Current (A)')
plt.ylabel('Efficiency (%)')
plt.title('HT-PEMFC Stack Efficiency')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()
plt.figure(figsize=(8, 5))
plt.plot(j_range, V_cell, label='Cell Voltage (V)')
plt.xlabel('Current Density (A/cm²)')
plt.ylabel('Voltage (V)')
plt.title('HT-PEMFC Cell Voltage vs Current Density')
plt.grid(True)
plt.legend()

```

```

plt.tight_layout()
plt.show()
power_density = j_range * V_cell # W/cm2
plt.figure(figsize=(8, 5))
plt.plot(j_range, power_density, color='green', label='Power Density (W/cm2)')
plt.xlabel('Current Density (A/cm2)')
plt.ylabel('Power Density (W/cm2)')
plt.title('HT-PEMFC Power Density vs Current Density')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()

# i) Plot effects of hydrogen concentrations
h2_concs = [0.5, 0.7, 1.0] # 50%, 70%, 100%
for conc in h2_concs:
    PH2_out_conc = PH2_out * conc
    E_nernst_conc = E0 - (R * T_fc / (2 * F)) * np.log((PH2_out_conc * PO2**0.5) /
P_H2O)
    V_cell_conc = []
    power_density_conc = []
    for j in j_range:
        eta_act = solve_eta_act(j, T_fc, j0, alpha_a, alpha_c)
        eta_ohmic = j * R_ohmic
        eta_conc = -(R * T_fc / (n_e * F)) * np.log(1 - j / j_lim) if j < j_lim else np.inf
        V = E_nernst_conc - eta_act - eta_ohmic - eta_conc
        V_cell_conc.append(V)
        power_density_conc.append(j * V) # W/cm2
    plt.plot(j_range, V_cell_conc, label=f'Voltage (H2={int(conc*100)}%)')

```

```

plt.plot(j_range, power_density_conc, '--', label=f'Power Density
(H2={int(conc*100)}%)')
plt.xlabel('Current Density (A/cm²)')
plt.ylabel('Voltage (V) / Power Density (W/cm²)')
plt.title('Effects of Hydrogen Concentration on HT-PEMFC Performance')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()

# -----
# Integrated MSR + HT-PEMFC efficiency
# -----

from scipy.interpolate import interp1d

# 1) Build a smooth V(j) interpolant from computed I–V curve
V_of_j = interp1d(j_range, V_cell, kind="cubic", fill_value="extrapolate")

# 2) Sweep current density up to modeled limit
j_sweep = np.linspace(0.02, min(0.30, np.max(j_range)), 120) # A/cm² (avoid j=0)

# 3) Parameterizations
F = 96485.0 # C/mol
LHV_H2 = 240e3 # J/mol
LHV_CH3OH = 638e3 # J/mol

# Hydrogen utilization def util_H2(x, u_low=0.70, u_high=0.85):
    return np.clip(u_low + (u_high - u_low) * x, 0.50, 0.95)

# Reformer efficiency
def eta_reformer(x, eta0=system_efficiency, slope=-0.03):
    return np.clip(eta0 + slope * x, 0.65, 0.90)

# Auxiliaries: fixed floor + load-proportional term (kW)
def P_aux_kW(P_gross_kW, P_fixed=1.5, frac=0.02):

```

```

    return P_fixed + frac * P_gross_kW

# 4) Compute arrays
P_gross_kW = []    # gross electrical power from stack
P_net_kW = []      # after auxiliaries
eta_int = []       # integrated efficiency (%)
P_aux_arr = []     # auxiliaries (kW)
# Rated power for normalisation and plotting
P_gross_tmp = []
for j in j_sweep:
    V = float(V_of_j(j))
    I_cell_A = j * A_cell_cm2          # A per cell
    P_stack_kW = (I_cell_A * V * n_cells) / 1000.0
    P_gross_tmp.append(P_stack_kW)
P Rated = max(P_gross_tmp) if len(P_gross_tmp) else 160.0

for j in j_sweep:
    # Electrochemistry
    V = float(V_of_j(j))
    I_cell_A = j * A_cell_cm2          # A per cell
    P_stack_kW = (I_cell_A * V * n_cells) / 1000.0 # gross kW
    # Normalised load
    x = P_stack_kW / P Rated
    # Hydrogen demand from current (include utilisation & purge)
    U = util_H2(x)                      # fractional utilisation
    H2_mol_s = (I_cell_A * n_cells) / (2.0 * F) # stoich H2 (mol/s) for the current
    H2_supply_mol_s = H2_mol_s / max(U, 1e-6) # supply needed given utilisation
    # Fuel energy in: methanol LHV rate computed via reformer efficiency
    # H2 LHV out from reformer = H2_supply_mol_s * LHV_H2
    eta_ref = eta_reformer(x)
    MeOH_LHV_in_W = (H2_supply_mol_s * LHV_H2) / max(eta_ref, 1e-6) # W

```

```

MeOH_LHV_in_kW = MeOH_LHV_in_W / 1000.0
# Auxiliaries and net power
P_aux = P_aux_kW(P_stack_kW)
P_net = max(P_stack_kW - P_aux, 0.0)
# Integrated efficiency (net electric / methanol LHV in)
eff = (P_net / MeOH_LHV_in_kW) * 100.0 if MeOH_LHV_in_kW > 0 else 0.0
P_gross_kW.append(P_stack_kW)
P_net_kW.append(P_net)
P_aux_arr.append(P_aux)
eta_int.append(eff)

P_gross_kW = np.array(P_gross_kW)
P_net_kW = np.array(P_net_kW)
eta_int = np.array(eta_int)
P_aux_arr = np.array(P_aux_arr)
# 5) Plot: integrated efficiency vs gross power
plt.figure(figsize=(8,5))
plt.plot(P_gross_kW, eta_int, lw=2, label='Integrated Efficiency')
plt.xlabel('Gross Stack Power (kW)')
plt.ylabel('Energy Efficiency (%)')
plt.title('Integrated MSR + HT-PEMFC Efficiency')
plt.grid(True); plt.legend(); plt.tight_layout(); plt.show()
# Show auxiliaries and net power for diagnostics
plt.figure(figsize=(8,5))
plt.plot(P_gross_kW, P_net_kW, label='Net Power (kW)')
plt.plot(P_gross_kW, P_aux_arr, label='Aux Load (kW)', linestyle='--')
plt.xlabel('Gross Stack Power (kW)')
plt.ylabel('Power (kW)')
plt.title('Gross vs Net Power and Auxiliary Loads')
plt.grid(True); plt.legend(); plt.tight_layout(); plt.show()

```

```
# Print peak efficiency operating point
i_peak = int(np.argmax(eta_int))
print(f"Peak    integrated    efficiency:    {eta_int[i_peak]:.1f}%    at    gross
{P_gross_kW[i_peak]:.1f} kW "
      f"(net {P_net_kW[i_peak]:.1f} kW, aux {P_aux_arr[i_peak]:.1f} kW)")
```

Appendix 9: Market-driven (Baseline) Techno-Economic Assessment Modelling Code

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm, uniform # For Monte Carlo distributions

# Assumptions based on 2025 forecasts
annual_energy_mwh = 39000 # MWh/year
lifetime_years = 25
discount_rate = 0.05
power_ht_kw = 6100
power_conv_kw = 6500
lhv_methanol_kwh_kg = 5.53
lhv_diesel_kwh_kg = 11.1
overall_eff_ht = 0.55
eff_conv = 0.40 # Realistic marine diesel efficiency

# CAPEX ($/kW)
capex_ht_per_kw = 1649.4
capex_conv_per_kw = 538.55
capex_ht_total = capex_ht_per_kw * power_ht_kw
capex_conv_total = capex_conv_per_kw * power_conv_kw

# OPEX maintenance ($/kW/year base)
maint_ht_per_kw_year_base = 32.33
maint_conv_per_kw_year_base = 10.77

# Annual maintenance growth rate
maint_growth_rate = 0.01 # 1% per year

# Fuel prices ($/tonne base)
methanol_prices = {'grey': 350, 'blue': 550, 'bio-MeOH': 1193, 'e-methanol': 2238}
fuel_prices = {'HFO': 442, 'MGO': 780}

# Fuel escalation rates (% per year, pathway-specific)
fuel_escalation_rates = {'grey': 0.05, 'blue': 0.025, 'bio-MeOH': 0.005, 'e-methanol': 0.001, 'HFO': 0.08, 'MGO': 0.08} # Higher for grey, lower for bio and e-methanol

# Annual fuel consumption (tonnes/year base, at year 1 efficiency)
annual_fuel_ht_kg = annual_energy_mwh * 1000 / (overall_eff_ht * lhv_methanol_kwh_kg)
annual_fuel_ht_tonnes = annual_fuel_ht_kg / 1000
```

```

annual_fuel_conv_kg = annual_energy_mwh * 1000 / (eff_conv *
lhv_diesel_kwh_kg)
annual_fuel_conv_tonnes = annual_fuel_conv_kg / 1000

# Efficiency degradation rate (% per year, for HT-PEMFC only)
eff_degradation_rate_ht = 0.005 # 0.5% per year degradation

# Emissions factors (tCO2eq/t fuel, midpoint WtT)
emission_factors = {'grey': 2.1, 'blue': 1.91, 'bio-MeOH': -0.796, 'e-methanol': 0.077,
'HFO': 3.789, 'MGO': 3.962} # Similar emission factors as in LCA analysis

# Functions
def npv(cashflows, rate):
    return sum(cf / (1 + rate)**t for t, cf in enumerate(cashflows, start=1))

def calculate_tco(capex, maint_base, maint_growth_rate, fuel_base_price,
fuel_escalation, eff_base, eff_degradation_rate, annual_fuel_tonnes_year1,
lhv_kwh_kg):
    annual_costs = []
    current_eff = eff_base
    current_maint = maint_base
    current_fuel_price = fuel_base_price
    for year in range(1, lifetime_years + 1):
        # Apply degradation to efficiency (increases fuel consumption)
        fuel_tonnes_year = annual_fuel_tonnes_year1 / (current_eff / eff_base) #
Adjusted fuel for degraded eff
        fuel_cost_year = fuel_tonnes_year * current_fuel_price
        maint_cost_year = current_maint
        annual_costs.append(maint_cost_year + fuel_cost_year)

        # Update for next year
        current_eff = max(current_eff * (1 - eff_degradation_rate), 0.3) # Cap at 30%
min eff
        current_maint *= (1 + maint_growth_rate)
        current_fuel_price *= (1 + fuel_escalation)

    npv_opex_fuel = npv(annual_costs, discount_rate)
    return capex + npv_opex_fuel

def calculate_lcoe(capex, maint_base, maint_growth_rate, fuel_base_price,
fuel_escalation, eff_base, eff_degradation_rate, annual_fuel_tonnes_year1,
lhv_kwh_kg):
    annual_costs = []
    annual_energies = []
    current_eff = eff_base

```

```

current_maint = maint_base
current_fuel_price = fuel_base_price
for year in range(1, lifetime_years + 1):
    # Adjusted energy output due to degradation
    energy_year_mwh = annual_energy_mwh * (current_eff / eff_base)
    fuel_tonnes_year = energy_year_mwh / (current_eff * lhv_kwh_kg) #
Consistent with degradation
    fuel_cost_year = fuel_tonnes_year * current_fuel_price
    maint_cost_year = current_maint
    annual_costs.append(maint_cost_year + fuel_cost_year)
    annual_energies.append(energy_year_mwh)

    # Update
    current_eff = max(current_eff * (1 - eff_degradation_rate), 0.3)
    current_maint *= (1 + maint_growth_rate)
    current_fuel_price *= (1 + fuel_escalation)

npv_costs = capex + npv(annual_costs, discount_rate)
npv_energy = npv(annual_energies, discount_rate)
return (npv_costs / npv_energy) if npv_energy > 0 else np.inf

def calculate_payback(extra_capex, annual_savings_list, rate,
max_years=lifetime_years):
    cumulative = 0
    num_years = len(annual_savings_list)
    for year in range(1, num_years + 1):
        discounted_savings = annual_savings_list[year-1] / (1 + rate)**year
        cumulative += discounted_savings
        if cumulative >= extra_capex:
            return year
    return num_years # Return lifetime if not paid back

def calculate_emissions_per_mwh(annual_fuel_tonnes_year1, eff_base,
eff_degradation_rate, emission_factor, lhv_kwh_kg):
    total_emissions = 0
    total_energy_mwh = 0
    current_eff = eff_base
    for year in range(1, lifetime_years + 1):
        energy_year_mwh = annual_energy_mwh * (current_eff / eff_base)
        fuel_tonnes_year = energy_year_mwh * 1000 / (current_eff * lhv_kwh_kg)
        emissions_year = fuel_tonnes_year * emission_factor
        total_emissions += emissions_year
        total_energy_mwh += energy_year_mwh
        current_eff = max(current_eff * (1 - eff_degradation_rate), 0.3)
    return total_emissions / total_energy_mwh if total_energy_mwh > 0 else np.inf

```

```

# Precompute annual savings lists for payback (vs HFO baseline)
annual_savings_lists = {}
conv_hfo_annual_costs = []
conv_hfo_current_maint = maint_conv_per_kw_year_base * power_conv_kw
conv_hfo_current_fuel_price = fuel_prices['HFO']
conv_hfo_current_eff = eff_conv # No degradation for conventional
for year in range(1, lifetime_years + 1):
    fuel_tonnes_year_conv = annual_energy_mwh * 1000 / (conv_hfo_current_eff *
lhv_diesel_kwh_kg)
    fuel_cost_year_conv = fuel_tonnes_year_conv * conv_hfo_current_fuel_price
    maint_cost_year_conv = conv_hfo_current_maint
    conv_hfo_annual_costs.append(maint_cost_year_conv + fuel_cost_year_conv)

    conv_hfo_current_maint *= (1 + maint_growth_rate)
    conv_hfo_current_fuel_price *= (1 + fuel_escalation_rates['HFO'])
    conv_hfo_current_eff = max(conv_hfo_current_eff * (1 - 0.002), 0.3) # 0.2%
degradation for conv

# Compute for HT-PEMFC pathways
results = {}
for meth_type, price in methanol_prices.items():
    annual_costs_ht = []
    current_maint_ht = maint_ht_per_kw_year_base * power_ht_kw
    current_fuel_price_ht = price
    current_eff_ht = overall_eff_ht
    for year in range(1, lifetime_years + 1):
        fuel_tonnes_year_ht = annual_energy_mwh * 1000 / (current_eff_ht *
lhv_methanol_kwh_kg)
        fuel_cost_year_ht = fuel_tonnes_year_ht * current_fuel_price_ht
        maint_cost_year_ht = current_maint_ht
        annual_costs_ht.append(maint_cost_year_ht + fuel_cost_year_ht)

        current_maint_ht *= (1 + maint_growth_rate)
        current_fuel_price_ht *= (1 + fuel_escalation_rates.get(meth_type, 0.03)) #
Default 3%
        current_eff_ht = max(current_eff_ht * (1 - eff_degradation_rate_ht), 0.3)

    tco_ht = calculate_tco(capex_ht_total, maint_ht_per_kw_year_base *
power_ht_kw, maint_growth_rate, price, fuel_escalation_rates.get(meth_type, 0.03),
overall_eff_ht, eff_degradation_rate_ht, annual_fuel_ht_tonnes,
lhv_methanol_kwh_kg)
    lcoe_ht = calculate_lcoe(capex_ht_total, maint_ht_per_kw_year_base *
power_ht_kw, maint_growth_rate, price, fuel_escalation_rates.get(meth_type, 0.03),

```

```

overall_eff_ht, eff_degradation_rate_ht, annual_fuel_ht_tonnes,
lhv_methanol_kwh_kg)

    annual_savings_ht = [conv_hfo_annual_costs[y-1] - annual_costs_ht[y-1] for y in
range(1, lifetime_years + 1)]
    payback_ht = calculate_payback(capex_ht_total - capex_conv_total,
annual_savings_ht, discount_rate)

    emissions_per_mwh_ht = calculate_emissions_per_mwh(annual_fuel_ht_tonnes,
overall_eff_ht, eff_degradation_rate_ht, emission_factors[meth_type],
lhv_methanol_kwh_kg)

    results[f'HT-PEMFC_{meth_type}'] = {'TCO ($M)': round(tco_ht / 1e6, 2),
'LCOE ($/MWh)': round(lcoe_ht, 2), 'Payback vs. HFO (years)': payback_ht if
payback_ht < lifetime_years else 'N/A', 'Emissions (tCO2eq/MWh)':
round(emissions_per_mwh_ht, 3)}

# Compute for Conventional pathways
for fuel_type, price in fuel_prices.items():
    annual_costs_conv = []
    current_maint_conv = maint_conv_per_kw_year_base * power_conv_kw
    current_fuel_price_conv = price
    current_eff_conv = eff_conv
    for year in range(1, lifetime_years + 1):
        fuel_tonnes_year_conv = annual_energy_mwh * 1000 / (current_eff_conv *
lhv_diesel_kwh_kg)
        fuel_cost_year_conv = fuel_tonnes_year_conv * current_fuel_price_conv
        maint_cost_year_conv = current_maint_conv
        annual_costs_conv.append(maint_cost_year_conv + fuel_cost_year_conv)

        current_maint_conv *= (1 + maint_growth_rate)
        current_fuel_price_conv *= (1 + fuel_escalation_rates[fuel_type])
        current_eff_conv = max(current_eff_conv * (1 - 0.002), 0.3) # 0.2%
degradation

    tco_conv = calculate_tco(capex_conv_total, maint_conv_per_kw_year_base *
power_conv_kw, maint_growth_rate, price, fuel_escalation_rates[fuel_type],
eff_conv, 0.002, annual_fuel_conv_tonnes, lhv_diesel_kwh_kg)
    lcoe_conv = calculate_lcoe(capex_conv_total, maint_conv_per_kw_year_base *
power_conv_kw, maint_growth_rate, price, fuel_escalation_rates[fuel_type],
eff_conv, 0.002, annual_fuel_conv_tonnes, lhv_diesel_kwh_kg)

    emissions_per_mwh_conv =
calculate_emissions_per_mwh(annual_fuel_conv_tonnes, eff_conv, 0.002,
emission_factors[fuel_type], lhv_diesel_kwh_kg)

```

```

    results[f'Conventional_{fuel_type}'] = {'TCO ($M)': round(tco_conv / 1e6, 2),
'LCOE ($/MWh)': round(lcoe_conv, 2), 'Emissions (tCO2eq/MWh)':
round(emissions_per_mwh_conv, 3)}

# Monte Carlo Simulation for Uncertainty (10,000 iterations)
num_iterations = 10000
mc_results = {scenario: {'TCO': [], 'LCOE': [], 'Payback': []} for scenario in
results.keys() if 'HT-PEMFC' in scenario}

for i in range(num_iterations):
    # Random perturbations (e.g., normal distribution for efficiency, uniform for
prices)
    eff_ht_mc = np.clip(norm.rvs(overall_eff_ht, 0.02), 0.3, 0.6) # Mean 0.55, SD
0.02
    capex_ht_mc = uniform.rvs(capex_ht_total * 0.9, capex_ht_total * 0.2) # ±10%
    fuel_price_mc = {k: uniform.rvs(v * 0.9, v * 0.2) for k, v in
methanol_prices.items()} # ±10%

    for meth_type in methanol_prices.keys():
        tco_ht_mc = calculate_tco(capex_ht_mc, maint_ht_per_kw_year_base *
power_ht_kw, maint_growth_rate, fuel_price_mc[meth_type],
fuel_escalation_rates.get(meth_type, 0.03), eff_ht_mc, eff_degradation_rate_ht,
annual_fuel_ht_tonnes, lhv_methanol_kwh_kg)
        lcoe_ht_mc = calculate_lcoe(capex_ht_mc, maint_ht_per_kw_year_base *
power_ht_kw, maint_growth_rate, fuel_price_mc[meth_type],
fuel_escalation_rates.get(meth_type, 0.03), eff_ht_mc, eff_degradation_rate_ht,
annual_fuel_ht_tonnes, lhv_methanol_kwh_kg)

        annual_costs_ht_mc = []
        current_eff_ht_mc = eff_ht_mc
        current_fuel_price_ht_mc = fuel_price_mc[meth_type]
        current_maint_ht_mc = maint_ht_per_kw_year_base * power_ht_kw
        for year in range(1, lifetime_years + 1):
            fuel_tonnes_year_ht_mc = annual_energy_mwh * 1000 / (current_eff_ht_mc
* lhv_methanol_kwh_kg)
            fuel_cost_year_ht_mc = fuel_tonnes_year_ht_mc * current_fuel_price_ht_mc
            maint_cost_year_ht_mc = current_maint_ht_mc
            annual_costs_ht_mc.append(maint_cost_year_ht_mc +
fuel_cost_year_ht_mc)

            current_eff_ht_mc = max(current_eff_ht_mc * (1 - eff_degradation_rate_ht),
0.3)
            current_fuel_price_ht_mc *= (1 + fuel_escalation_rates.get(meth_type,
0.03))

```

```

        current_maint_ht_mc *= (1 + maint_growth_rate)

        annual_savings_ht_mc = [conv_hfo_annual_costs[y-1] - annual_costs_ht_mc[y-
1] for y in range(1, lifetime_years + 1)]
        payback_ht_mc = calculate_payback(capex_ht_mc - capex_conv_total,
annual_savings_ht_mc, discount_rate)

        mc_results[f'HT-PEMFC_{meth_type}']['TCO'].append(tco_ht_mc / 1e6)
        mc_results[f'HT-PEMFC_{meth_type}']['LCOE'].append(lcoe_ht_mc)
        mc_results[f'HT-PEMFC_{meth_type}']['Payback'].append(payback_ht_mc if
payback_ht_mc < lifetime_years else lifetime_years)

# Monte Carlo results (mean and 95% CI)
for scenario, metrics in mc_results.items():
    for metric, values in metrics.items():
        mean = np.mean(values)
        ci_low, ci_high = np.percentile(values, [2.5, 97.5])
        print(f'{scenario} {metric}: Mean = {mean:.2f}, 95% CI = [{ci_low:.2f},
{ci_high:.2f}]")

# Plots
scenarios = list(results.keys())
tco_values = [results[s]['TCO ($M)'] for s in scenarios]
plt.figure(figsize=(10, 6))
plt.bar(scenarios, tco_values)
plt.ylabel('TCO ($M over 25 Years)')
plt.title('Total Cost of Ownership Comparison')
plt.xticks(rotation=45, ha='right')
plt.grid(True)
plt.tight_layout()
plt.show()

lcoe_values = [results[s]['LCOE ($/MWh)'] for s in scenarios]
plt.figure(figsize=(10, 6))
plt.bar(scenarios, lcoe_values)
plt.ylabel('LCOE ($/MWh over 25 Years)')
plt.title('Levelized Cost of Energy Comparison')
plt.xticks(rotation=45, ha='right')
plt.grid(True)
plt.tight_layout()
plt.show()

meth_types = [k.split('_')[1] for k in results if 'HT-PEMFC' in k]

```

```

payback_values = [results[f'HT-PEMFC_{meth}']['Payback vs. HFO (years)'] if
isinstance(results[f'HT-PEMFC_{meth}']['Payback vs. HFO (years)'], int) else
lifetime_years for meth in meth_types]
plt.figure(figsize=(10, 6))
plt.bar(meth_types, payback_values)
plt.ylabel('Discounted Payback Period (years)')
plt.title('Payback Period of Methanol Pathways vs. HFO')
plt.grid(True)
plt.tight_layout()
plt.show()

emissions_values = [results[s]['Emissions (tCO2eq/MWh)'] for s in scenarios]
plt.figure(figsize=(10, 6))
plt.bar(scenarios, emissions_values)
plt.ylabel('Emissions (tCO2eq/MWh over Lifetime)')
plt.title('Emissions per MWh Comparison')
plt.xticks(rotation=45, ha='right')
plt.grid(True)
plt.tight_layout()
plt.show()

metrics_mc = {'TCO': 'TCO ($M)', 'LCOE': 'LCOE ($/MWh)', 'Payback': 'Payback
(years)', 'Emissions': 'Emissions (tCO2eq/MWh)', 'CarbonLevy': 'Carbon Levy
($M)', 'Subsidy': 'Subsidy ($M)'}

for m,label in metrics_mc.items():
    plt.figure(figsize=(10,6))
    for fuel,data in mc_results.items():
        arr = [x for x in data[m] if not np.isnan(x)]
        if len(arr)>0:
            plt.hist(arr, bins=50, alpha=0.5, density=True, label=fuel)
    plt.xlabel(label); plt.ylabel("Density"); plt.title(f"Monte Carlo {label}
distributions")
    plt.legend(); plt.tight_layout(); plt.show()

```

Appendix 10: Policy-Driven Techno-Economic Assessment Modelling Code

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm
import pandas as pd

# -----
# Model assumptions
# -----
annual_energy_mwh = 39000
lifetime_years = 25
discount_rate = 0.05
power_ht_kw = 6100
power_conv_kw = 6100
lhv_methanol_kwh_kg = 5.53
lhv_diesel_kwh_kg = 11.1
lhv_mgo_kwh_kg = 11.86
overall_eff_ht = 0.55
eff_conv = 0.40
eff_degradation_rate_ht = 0.015
eff_degradation_conv = 0.002

# CAPEX ($/kW)
capex_ht_per_kw = 1649.4
capex_conv_per_kw = 538.55
capex_ht_total = capex_ht_per_kw * power_ht_kw
capex_conv_total = capex_conv_per_kw * power_conv_kw

# OPEX maintenance (base $/year)
maint_ht_per_kw_year_base = 32.33
maint_conv_per_kw_year_base = 10.77
maint_growth_rate = 0.01

# Fuel prices ($/t)
methanol_prices = {'grey': 350, 'blue': 550, 'bio-MeOH': 1193, 'e-methanol': 2238}
fuel_prices = {'HFO': 442, 'MGO': 780}

# Escalation rates
fuel_escalation_rates = {
    'grey': 0.05, 'blue': 0.025, 'bio-MeOH': 0.005, 'e-methanol': 0.001,
    'HFO': 0.08, 'MGO': 0.08
}
```

```

# Emission factors (tCO2eq/t fuel)
emission_factors = {
    'grey': 2.1, 'blue': 1.91, 'bio-MeOH': -0.796, 'e-methanol': 0.095,
    'HFO': 3.789, 'MGO': 3.962
}

START_YEAR = 2025

# -----
# Helper functions
# -----
def get_subsidy_rate(fuel_type, calendar_year, policy_enabled=True):
    if not policy_enabled:
        return 0.0
    if fuel_type == 'e-methanol':
        return 64 if calendar_year < 2034 else 760
    elif fuel_type == 'bio-MeOH':
        return 180
    return 0.0

def npv(cashflows, rate):
    return sum(cf / (1 + rate)**t for t, cf in enumerate(cashflows, start=1))

def build_annual_streams(eff_base, eff_degradation_rate,
                        maint_base, maint_growth,
                        fuel_price_base, fuel_escalation,
                        lhv_kwh_kg, emission_factor,
                        levy_rate=100, fuel_type=None,
                        policy_enabled=True):
    energies = np.full(lifetime_years, annual_energy_mwh, dtype=float)
    fuel_tonnes = np.zeros(lifetime_years)
    fuel_costs = np.zeros(lifetime_years)
    maint_costs = np.zeros(lifetime_years)
    emissions = np.zeros(lifetime_years)
    carbon_levy_costs = np.zeros(lifetime_years)
    subsidy_rev = np.zeros(lifetime_years)

    eff = eff_base
    fuel_price = fuel_price_base
    maint = maint_base

    for i in range(lifetime_years):
        calendar_year = START_YEAR + i
        fuel_kg = energies[i] * 1000.0 / (eff * lhv_kwh_kg)
        fuel_t = fuel_kg / 1000.0

```

```

fuel_tonnes[i] = fuel_t

fuel_costs[i] = fuel_t * fuel_price
maint_costs[i] = maint
emissions[i] = fuel_t * emission_factor

taxable_emissions = emissions[i]
carbon_levy_costs[i] = taxable_emissions * levy_rate

subsidy_rate = get_subsidy_rate(fuel_type, calendar_year, policy_enabled) if
fuel_type in ['bio-MeOH', 'e-methanol'] else 0.0
subsidy_rev[i] = fuel_t * subsidy_rate

eff = max(eff * (1 - eff_degradation_rate), 0.3)
fuel_price *= (1 + fuel_escalation)
maint *= (1 + maint_growth)

return {
    'energy_mwh': energies,
    'fuel_tonnes': fuel_tonnes,
    'fuel_costs': fuel_costs,
    'maint_costs': maint_costs,
    'emissions_tCO2': emissions,
    'carbon_levy_$': carbon_levy_costs,
    'subsidy_$': subsidy_rev
}

def calc_tco(capex, streams, discount_rate):
    annual_opex = streams['fuel_costs'] + streams['maint_costs'] +
streams['carbon_levy_$'] - streams['subsidy_$']
    return capex + npv(annual_opex, discount_rate)

def calc_lcoe(capex, streams, discount_rate, residual_rate=0.0):
    annual_opex = streams['fuel_costs'] + streams['maint_costs'] +
streams['carbon_levy_$'] - streams['subsidy_$']
    npv_costs = capex + npv(annual_opex, discount_rate)
    npv_energy = npv(streams['energy_mwh'], discount_rate)
    residual_value = capex * residual_rate / (1 + discount_rate)**lifetime_years if
residual_rate else 0.0
    return (npv_costs - residual_value) / npv_energy if npv_energy > 0 else np.inf

def calc_emissions_per_mwh(streams):
    return streams['emissions_tCO2'].sum() / streams['energy_mwh'].sum()

```

```

def calc_discounted_payback(extra_capex, baseline_streams, candidate_streams,
discount_rate):
    baseline_costs = baseline_streams['fuel_costs'] + baseline_streams['maint_costs']
+ baseline_streams['carbon_levy_$'] - baseline_streams['subsidy_$']
    candidate_costs = candidate_streams['fuel_costs'] +
candidate_streams['maint_costs'] + candidate_streams['carbon_levy_$'] -
candidate_streams['subsidy_$']
    savings = baseline_costs - candidate_costs
    cumulative = 0.0
    for y, s in enumerate(savings, start=1):
        cumulative += s / (1 + discount_rate)**y
        if cumulative >= extra_capex:
            return y
    return lifetime_years + 1

# -----
# Deterministic run function
# -----
def run_deterministic(levy_rate):
    results = {}

    conv_hfo_streams = build_annual_streams(
        eff_base=eff_conv,
        eff_degradation_rate=eff_degradation_conv,
        maint_base=maint_conv_per_kw_year_base * power_conv_kw,
        maint_growth=maint_growth_rate,
        fuel_price_base=fuel_prices['HFO'],
        fuel_escalation=fuel_escalation_rates['HFO'],
        lhv_kwh_kg=lvh_diesel_kwh_kg,
        emission_factor=emission_factors['HFO'],
        levy_rate=levy_rate,
        fuel_type='HFO'
    )

    conv_mgo_streams = build_annual_streams(
        eff_base=eff_conv,
        eff_degradation_rate=eff_degradation_conv,
        maint_base=maint_conv_per_kw_year_base * power_conv_kw,
        maint_growth=maint_growth_rate,
        fuel_price_base=fuel_prices['MGO'],
        fuel_escalation=fuel_escalation_rates['MGO'],
        lhv_kwh_kg=lvh_mgo_kwh_kg,
        emission_factor=emission_factors['MGO'],
        levy_rate=levy_rate,
        fuel_type='MGO'

```

```

)

for meth, price in methanol_prices.items():
    streams = build_annual_streams(
        overall_eff_ht, eff_degradation_rate_ht,
        maint_ht_per_kw_year_base * power_ht_kw, maint_growth_rate,
        price, fuel_escalation_rates[meth],
        lhv_methanol_kwh_kg, emission_factors[meth],
        levy_rate=levy_rate,
        fuel_type=meth, policy_enabled=True
    )
    tco = calc_tco(capex_ht_total, streams, discount_rate)
    lcoe = calc_lcoe(capex_ht_total, streams, discount_rate)
    emissions = calc_emissions_per_mwh(streams)
    payback = calc_discounted_payback(capex_ht_total - capex_conv_total,
conv_hfo_streams, streams, discount_rate)

    results[f'HT-PEMFC_{meth}'] = {
        'TCO ($M)': round(tco/1e6, 3),
        'LCOE ($/MWh)': round(lcoe, 2),
        'Payback (years)': payback,
        'Emissions (tCO2eq/MWh)': round(emissions, 4)
    }

    results['HFO'] = {
        'TCO ($M)': round(calc_tco(capex_conv_total, conv_hfo_streams,
discount_rate)/1e6, 3),
        'LCOE ($/MWh)': round(calc_lcoe(capex_conv_total, conv_hfo_streams,
discount_rate), 2),
        'Emissions (tCO2eq/MWh)':
round(calc_emissions_per_mwh(conv_hfo_streams), 4)
    }
    results['MGO'] = {
        'TCO ($M)': round(calc_tco(capex_conv_total, conv_mgo_streams,
discount_rate)/1e6, 3),
        'LCOE ($/MWh)': round(calc_lcoe(capex_conv_total, conv_mgo_streams,
discount_rate), 2),
        'Emissions (tCO2eq/MWh)':
round(calc_emissions_per_mwh(conv_mgo_streams), 4)
    }

    return results

# -----
# Scenario loop and plotting

```

```

# -----
def run_and_plot(levy_rates=[100,200,300,400,500]):
    scenario_results = {}

    for levy in levy_rates:
        scenario_results[levy] = run_deterministic(levy)

    # Deterministic DataFrame
    det_rows = []
    for levy, res in scenario_results.items():
        for fuel, metrics in res.items():
            row = {"Levy": levy, "Fuel": fuel}
            row.update(metrics)
            det_rows.append(row)
    det_df = pd.DataFrame(det_rows)

    fuel_order = ['HFO', 'MGO'] + [f'HT-PEMFC_{k}' for k in ['grey', 'blue', 'bio-
MeOH', 'e-methanol']]
    det_df['Fuel'] = pd.Categorical(det_df['Fuel'], categories=fuel_order,
ordered=True)
    det_df = det_df.sort_values(['Fuel', 'Levy']).reset_index(drop=True)

    # Deterministic plots
    metrics_det = ['TCO ($M)', 'LCOE ($/MWh)', 'Payback (years)', 'Emissions
(tCO2eq/MWh)']
    for metric in metrics_det:
        plt.figure(figsize=(8,5))
        for fuel in det_df['Fuel'].cat.categories:
            subset = det_df[det_df['Fuel'] == fuel]
            if subset.empty: continue
            plt.plot(subset['Levy'], subset[metric], marker='o', label=fuel)
        plt.xlabel("Carbon Levy ($/tCO2eq)")
        plt.ylabel(metric)
        plt.title(f"{metric} vs Carbon Levy")
        plt.legend(bbox_to_anchor=(1.05, 1), loc='upper left', borderaxespad=0.)
        plt.grid(True)
        plt.tight_layout()
        plt.show()

if __name__ == "__main__":
    det_df = run_and_plot(levy_rates=[100,200,300,400,500])

```