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A multi-fuel pathway explorer tool for evaluating sustainable alternative fuels for the maritime sector

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ABSTRACT

In the maritime sector, sustainable alternative fuels derived from biological and non-biological origin such as hydrogen, ammonia, and methanol show high potential for novel propulsion technologies such as solid oxide fuel cells. Since transitioning to new fuels may require high investments, decision-makers and local municipalities need a systematic approach to identify the most relevant fuel pathways for their prerequisites. However, a modelling approach including fuel production, transport, demand, time-resolved supply rates for testing and comparing sustainable alternative fuels is still lacking. Here, a Python library called multi-fuel pathway explorer (MFPE) was developed for fuel-cell applications in the maritime sector. The library offers the possibility of rapid screening and modelling of high-potential pathways depending on the constituents of the target port environment, allowing for in-depth evaluation of technical details compared to commonly applied life-cycle assessment (LCA) or techno-economical assessment (TEA) tools. For demonstration, a case study was set up at the port of Rotterdam to evaluate fuel pathways by calculation of selected key performance indicators (KPIs). Results demonstrate that the model is applicable to complex multi-fuel systems to compare fuel pathways, identify system-level bottlenecks, and analyse time-resolved dependencies between fuel demand and supply along the pathway.

Keywords

Maritime sector defossilisation;
Power-to-X;
Solid oxide fuel cells;
Multi-fuel pathways;
Time-resolved simulation

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1 Introduction

The maritime industry is a significant contributor to global greenhouse gas (GHG) emissions, accounting for ~2.9% of all emissions, which is equivalent to ~1 billion tonnes of CO₂ attributed to human activities [1]. This substantial contribution underscores the urgent need for cleaner, more sustainable alternative fuel sources [2]. To reduce GHG emissions, the International Maritime Organization (IMO) has set ambitious goals, making it imperative to identify and adopt alternative maritime fuels [3].

However, the transition requires a balanced strategy combining technological enhancements, systemic optimisation, and comprehensive environmental impact assessments [4]. By integrating these elements, the maritime industry may have the chance to transition into a

new era combining operational efficiency and long-term economic and ecologic sustainability.

Apart from IMO, the European Union (EU) aims in the “FuelEU Maritime” regulation to transition maritime fuels towards renewable and low-carbon fuels and to substitute sources of energy until 2050. The current regulation applies to ships with a gross tonnage (GT) above 5,000 (including some exceptions) [5]. The targets are ambitious and specifically target the transition towards renewable fuels of non-biological origin (RFNBOs) apart from the other two main goals of lowering lifecycle GHG intensity and electrification of ships at berth starting 2025 [5].

For defossilization of the maritime shipping industry by introducing sustainable alternative fuels, the following fuels, hydrogen (H₂), ammonia (NH₃), and methanol (MeOH) are of high importance and can be combined

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with novel powertrain technologies such as solid oxide fuel cells (SOFC). Such systems are relatively versatile, allow scaling and can run with either of the above mentioned fuels [6]. Table 1 provides an overview of sustainable alternative fuels currently identified as important for the energy transition.

Green hydrogen, currently considered at technology readiness level (TRL) 7-9 is close to large scale commercialization while bio-hydrogen generally has lower maturity and is considered at TRL 4-7. While green hydrogen may have high process efficiencies of 60-80% [8], bio-hydrogen production is less efficient but utilizes and valorises waste [9].

Ammonia synthesized by the Haber-Bosch process is the most prominent example for the industrial revolution and its production is currently responsible for ~1% of global CO₂ emissions [10]. While its production is currently largely dependent on natural gas, green ammonia (TRL 5-7) is considered a promising alternative. However, waste utilization and recovery of ammonia

from waste and wastewater may also be a viable option for fuel provision (TRL 4-8).

Methanol produced from natural gas is currently in debate to be better derived from biogas upgrading (TRL 6-7) [11, 12].

While alternative fuels and production technologies are relatively well known and regulations are being issued by policy makers, energy planning research increasingly focuses on the availability of integrated and sector-coupled modelling approaches that provide evidence for aided infrastructure and technology choices for the part of energy system transition planning.

As part of the scope of IJSEPM and the Smart Energy Systems literature, it is clear that energy system analysis, feasibility assessment, electrification, power-to-X, flexibility, and integrated infrastructure planning are required for the future of energy system defossilisation in general and that includes the maritime sector [13-15]. Since fuel pathway choices in shipping are associated with long-term infrastructure and investment decisions,

Table 1: Sustainable alternative fuels, production process and feedstock as potential candidates for the maritime industry (not complete), ANNEX IX Part A/B refers to [7].

Category	Fuel	Production Process	Feedstock Type
Biofuels	Cellulosic Ethanol	Enzymatic hydrolysis fermentation	Annex IX Part A
Biofuels	Bio-Methanol**	Gasification synthesis	Annex IX Part A
Biofuels	Bio-LNG	Anaerobic digestion upgrading	Annex IX Part A
Biofuels	Bio-Hydrogen**	Biomass gasification shift	Annex IX Part A
Biofuels	Biodiesel (HVO)	Hydroprocessed esters and fatty acids (HEFA)	Annex IX Part B
Biofuels	FT-Diesel	Gasification + Fischer-Tropsch	Annex IX Part A
Biofuels	Bio-Ethanol	Fermentation	Annex IX Part A
Fossil fuels	LNG	Natural gas liquefaction	Fossil gas
Low-carbon fuel	Blue Hydrogen	Steam methane reforming CCS	Natural gas + CCS
Low-carbon fuel	Blue Ammonia	Blue hydrogen + Haber-Bosch	Natural gas + CCS
Recycled Fuels	Recovered Ammonia**	Ion exchange (NH ₄ ⁺)	Renewable electricity + Wastewater
Recycled Carbon Fuels	Waste-based carbon fuels	Plastic pyrolysis / gas fermentation	Fossil waste streams
RFNBO*	E-Methanol (Green Methanol)	Electrolysis CO ₂ synthesis	Renewable electricity + CO ₂
RFNBO	E-Ammonia (Green Ammonia)	Electrolysis + Haber-Bosch	Renewable electricity + N ₂
RFNBO	E-Diesel	Electrolysis + FT synthesis	Renewable electricity + CO ₂
RFNBO	E-Methane	Methanation (Sabatier)	Renewable electricity + CO ₂
RFNBO	Green hydrogen**	Water electrolysis	Renewable electricity
RFNBO	Green ammonia**	Green hydrogen + Haber-Bosch	Renewable electricity

*Renewable fuels of non-biological origin

**Fuels selected in this paper

decision-makers need a structured approach for early-stage comparison of their high-potentials to identify promising options before committing to more detailed analyses. Most of the existing tools address selected elements of maritime fuel-pathways in a fragmented manner, with narrow system boundaries, detailed datasets, or considerable modelling effort and they usually do not explicitly capture time-resolved system operation, e.g. [16-19].

With time-resolved data included, the physical dimension of the system, including storage sizing and infrastructure requirements, can be adjusted and stressed in sufficient detail, but this is still lacking in the available time-resolved models [20]. Meanwhile other possibilities contain or are mainly proprietary software packages, limiting transparency, accessibility, and adaptability to real-world problems [21-23].

This is particularly relevant for early-stage pathway assessment, where open-source tools offer a clear advantage by facilitating model extension, adaptation, and application to different use cases, while such flexibility is often restricted in proprietary or highly rigid modelling environments as utilized in [24-28]. While Hampp et al. utilize a time-resolved open modelling framework, their focus is mainly on the comparison of renewable energy import pathways based on costs of different chemical energy carriers, but they do not consider demand profiles or fuel utilization [29].

Here, we present a novel, open-source “Multi Fuel Pathway Explorer (MFPE)” modelling framework, intended as a screening tool to enable a rapid, time-resolved evaluation of alternative fuel pathways from feedstock until utilization. Its main advantage is in pre-selecting the most promising pathways for a specific set of boundary conditions through data-driven comparison and identifying key trade-offs, bottlenecks like infrastructure sizing, and pathway requirements early on.

This allows that the most relevant fuel pathways can subsequently be analysed in more detail with state-of-the-art tools and methods such as LCA [17], TEA [16], Aspen Plus [21], or GREET [24]. The MFPE framework further allows flexible integration and expansion of any parameterized fuel pathways, components, processes via a generic and modular pathway design, ensuring adaptability to future technological developments and any other fuel utilization technology or target demand profile.

2 Materials and methods

The design approach for the MFPE for fuel pathway evaluation is based on the following framework consisting of six main layers (A-F), summarized in Figure 1.

Initially, industrial fuel production technologies were defined (Figure 1-A), then fuel pathways were

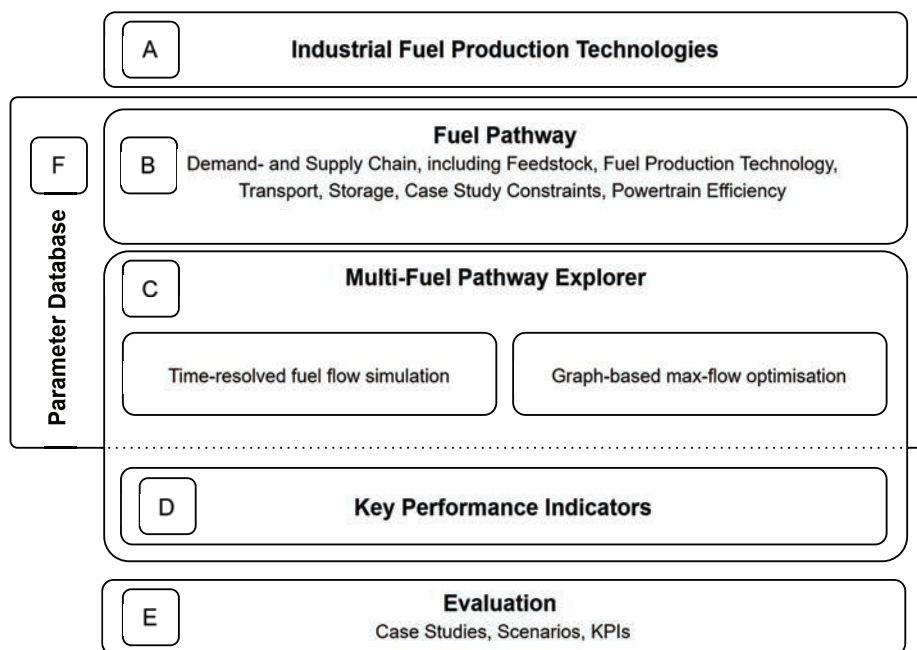


Figure 1: MFPE conceptual design approach.

developed (Figure 1-B) and parameterized in a database (Figure 1-F), including system parameters, flow sheets, process descriptions, pre- and post-conditions, acceptance criteria, case study demand, post-constituents, shipping fleet model, geographic location, environmental parameters, and other design inputs; pathway details are reported in [30].

A Python [31] library containing two modules was set up (Figure 1-C). The ‘Component’ module contains a base class and derived component classes (e.g. photovoltaic [PV], storage, port), which inherit from the base class. The ‘Pathway’ module connects components, handles the time-resolved flow simulation, and solves the graph-based max-flow problem each time-step while being the core part of the MFPE.

KPIs, including levelized costs of fuel (LCOF), well-to-wake (W2W) efficiency and TRL, were set up. Their

calculation was integrated on component-level and for the whole fuel pathway (Figure 1-D). While case study evaluation based on KPIs is not an integrated part of the MFPE, it can be carried out manually and user-specific with the provided data (Figure 1-E).

2.1 Fuel pathways, scenarios and case study

Fuel pathways for green and bio-hydrogen, green- and recovered ammonia, and bio-methanol including all relevant components required for the modelling approach were set up (Table 2) and parameterized using literature values. Cost functions for any components containing economic values were calculated on a 2020 reference year basis.

Pathway selection was based on the recommendations in the “FuelEU Maritime” Regulation with a strong focus on RFNBO fuels, however for comparison

Table 2: Overview of pathways, parameterization detail and scenarios as defined in [30].

Fuel Pathway	Details	Components
Pathway 1: Green Hydrogen (P1 GH2)	Renewable electricity (PV), PEM electrolyser; H ₂ transport by pipeline to port; short- and long-term storage integrated.	water purification unit, H ₂ tank storage, pipeline transport, port storage and decompression.
Scenarios	A: PV with grid connection, two storage tanks for short-term buffering, gaseous or liquified hydrogen as output B: PV with battery backup, one storage tank for short-term buffering, one salt cavern for seasonal storage, gaseous or liquified hydrogen as output	
Pathway 2: Bio-Hydrogen (P2 BH2)	Biomass gasification produces syngas converted to H ₂ ; Renewable electricity (PV + grid); fuel stored and transported to port.	Biomass feedstock supply, gasifier, gas cleaning unit, compression and storage, pipeline transport, port storage and decompression.
Scenarios^a	A: palm kernel shells, B: wood, C: pine forest, D: wheat straw	
Pathway 3: Green Ammonia (P3 GNH3)	H ₂ from PEM (see H2 UC 1) combined with N ₂ (air separation) in Haber–Bosch process; ammonia stored, pipeline to port.	PV system, PEM unit, H ₂ storage, Air Separation Unit (ASU), Haber–Bosch reactor, ammonia storage, pipeline transport to port, port storage.
Scenarios	PV with grid connection, two storage tanks for hydrogen, one storage tank for ammonia	
Pathway 4: Recovered Ammonia (P4 RNH3)	Nitrogen recovery via ion exchange from wastewater at different ammonium (NH ₄ ⁺) concentrations; ammonia is recovered, stored, and transported to port.	Wastewater feed unit, ion exchange reactor, regeneration system, renewable electricity (PV + grid), ammonia storage, pipeline transport, port storage.
Scenarios^b	A: municipal wastewater, low (40 mg N/L), B: municipal wastewater, high (100 mg N/L), C: industrial wastewater, low (356 mg N/L), D: industrial wastewater, high (594 mg N/L)	
Pathway 5: Bio-Methanol (P5 BMeOH)	Biomass is gasified to syngas and combined with green H ₂ for methanol synthesis; fuel stored and transported to port.	Biomass feed supply, gasifier + gas cleaning, H ₂ supply (PEM), methanol synthesis reactor, methanol storage, pipeline transport, port storage.
Scenarios^c	A: palm kernel shells, B: wood, C: pine forest, D: wheat straw	

^aPV with grid connection, two storage tanks for short-term buffering, but with varying feedstock A-D.

^bPV with grid connection, two storage tanks for ammonia, varying feeds, and ammonium nitrogen concentration.

^cPV with grid connection, hydrogen storage tank, methanol storage tank with varying feedstock for biomass gasification.

biofuels and waste recycled fuels were also included in this MFPE demonstration case study.

For modelling the fuel pathways presented in Table 2, a case study was designed for the port of Rotterdam, NL which is considered the biggest harbour in Europe with approx. 28,000 ocean-going vessels and approx. 92,000 inland vessels calling at the port every year [32].

About 250 km north-east of the port, in Zuidwending, NL salt caverns are situated which are suitable for hydrogen storage [33]. In addition to the storage, on-site production of green hydrogen in Zuidwending may be facilitated in the future by electrolysis using PV (potential approx. 900 - 1,050 kWh/m²/year) [34, 35].

Thus, for the case study the following prerequisites were set for defining an exemplary fuel demand profile: A small container vessel (i.e. Feeder Vessel) has an installed propulsion capacity of 10 MW. Based on a 75% average operational load, the effective propulsion power is 7.5 MW [36] and with an estimated average operating duration of 30 days between refuelling, the propulsion energy demand per fuelling cycle is calculated to be 5,400 MWh per fuelling trip.

For the case study, a supply rate of 30% of the propulsion energy demand for all ocean-going vessels calling at the port was set as target, translating into an average 0.96 ships per hour to arrive and need refuelling. This sets the model energy demand to 5,208 MWh/h, translating into a demand of 355, 2051, and 1958 t/h for hydrogen, ammonia, and methanol respectively.

2.2 Multi-Fuel Pathway Explorer development

The MFPE was developed as a Python library combining parameterized component-level models within a graph structure to a fully time-resolved system simulation enabling a quantitative evaluation of different alternative fuel pathways. The approach is reaching beyond conventional metrics to encompass crucial aspects within a fuel pathway such as fuel demand, electricity requisites, water consumption, LCOF and W2W efficiency. While the modular structure allows the integration of all major fuel pathway components, environmental impact assessment such as GHG emissions are not currently supported.

Unlike TEA, which identifies economic bottlenecks, the MFPE also enables the identification of technical bottlenecks along the fuel pathway [37]. Compared to a TEA approach, the MFPE includes a simplified economic representation, incorporating capital expenditure

(CAPEX) and operating expenses (OPEX) data for each component to calculate the LCOF across the entire fuel pathway [37]. The cost calculation is based on the simulation period, with operating costs scaled on an annual basis, including discounting and lifetime considerations.

For fuel pathway evaluation, KPIs are calculated as quantitative measures and are defined within a W2W scope, covering all stages from fuel production to its final use for ship propulsion. Component-level KPIs are determined and subsequently aggregated to evaluate system performance, bottlenecks, and support optimisation. For comparability, all KPIs are normalized for propulsion energy.

This includes: LCOF representing total lifetime cost of fuel generation, transport, storage, and use per unit of energy produced, the pathway efficiency based on components and overall W2W efficiencies, indicating total energy performance and potential for loss reduction, and TRL, measuring the maturity of technologies within the fuel pathway to guide investment and implementation decisions.

The MFPE Python library has been made accessible via an open-source Gitlab repository, where all equations and further explanation can be found [38].

2.2.1 Python library structure

The MFPE library structure is depicted in Figure 2 and comprises two modules, the 'Component' module containing the 'Component' base class and its derived specific component classes (e.g. 'Port' class, 'PV' class) while the 'Pathway' module contains the 'Pathway' class.

The 'Component' class is the fundamental building block for the fuel pathway. Each component represents a distinct element (input and output streams) within the fuel supply pathway and all specified component subclasses inherit from its base class. Depending on the subclass, the physical process is computed, and demand and supply is linked. Time-resolved data is logged for KPI calculation or structural optimisation of the pathway.

The 'Pathway' class is the central part of the MFPE, handles the construction of pathways and the interaction between different components, calculates the time-resolved flows using a time step of one hour and after the simulation aggregates the KPIs from all connected components in a postprocessing step.

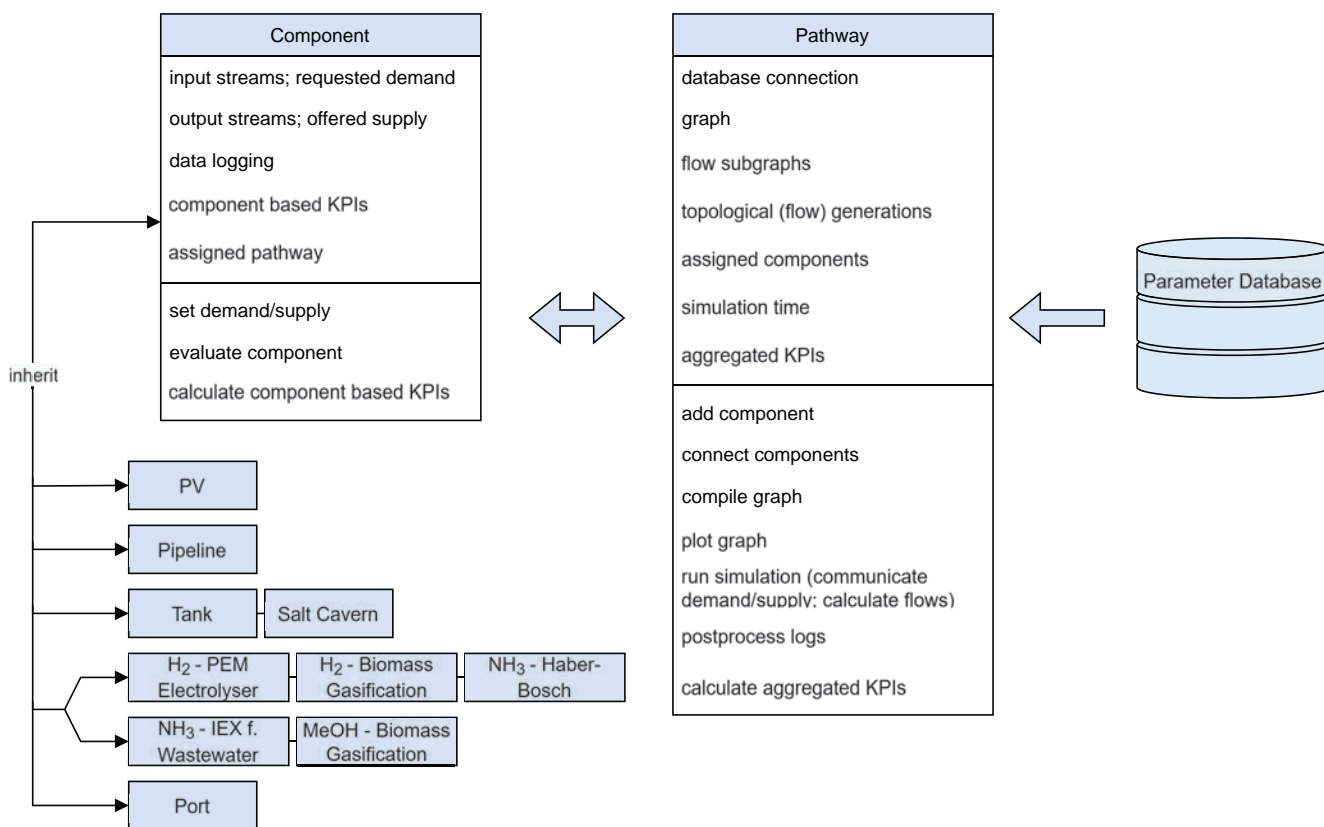


Figure 2: Class structure of the MFPE Python library (Diagram used from [39] with permission).

The parameter database provides the backbone of the MFPE, storing all parameters required for time-resolved flow calculations in the simulation and KPI calculation. Utilizing an SQLite database ensures efficient and reliable data management. The database connection is established within the ‘Pathway’ class, and all ‘Component’ subclasses can access it through the connection to their respective ‘Pathway’ instance.

2.2.2 Software design concept and modelling

Fuel pathways are modelled in the MFPE in two ways, (i) a time-resolved simulation of fuel flow, accounting for storage sizes, flow rates, and other dynamic variables based on the defined pathway, case study and scenario, and through (ii) KPI calculations, providing metrics to evaluate and optimise the performance of fuel pathways.

Graph data structures are used for fuel pathway design and max-flow optimisation. This allows fuel pathways to be represented and analysed while preserving design flexibility, which is implemented using the Python library NetworkX [40]. The graph representing a

fuel pathway consists of nodes or vertices, with nodes representing the pathway components (energy supply, fuel generation, transport, and storage), and edges between these nodes carrying information about the quantity being transferred (type, current mass flow).

Automatic determination of the computation sequence via topological ordering (Figure 3-A) is enabled via utilization of so-called directed acyclic graphs. This means that no closed loops are formed by following the directions within. Ordering produces a sequence of topologic generations (sets of nodes, that may be evaluated concurrently) respecting the direction of the edges and therefore ensures intact causality. Consequently, stage-wise analysis of flow behaviour, where information propagates forward through successive generations can be carried out.

Since the present work treats multiple quantities flowing in one graph that all need to be conserved separately, the graph is split up into quantity-specific subgraphs. Based on the subgraphs a set of auxiliary flow subgraphs is derived, where nodes are classified into supply nodes (those with outgoing edges) and demand

nodes (those with incoming edges), augmented with a synthetic super-source and super-sink.

The super-source is connected to all supply nodes via auxiliary edges, while the super-sink is connected to all demand nodes via auxiliary edges. These auxiliary edges have infinite capacity and serve as placeholders for assigning optimal supply/demand magnitudes during the flow simulation.

Finally, direct flow edges between supply and demand nodes are instantiated using capacity values that reflect node-level flow constraints. Specifically, the capacity of each internal edge is computed as the minimum of the maximum outgoing flow that a supply node can provide for the quantity and the maximum incoming flow that the connected demand node can accept. The resulting graphs are amenable to standard network flow algorithms, especially the max-flow algorithm, that is used for flow calculation [39].

This approach enables flexible pathway construction, allowing multiple quantities in one graph and unrestricted pathway design, provided no loops occur and the graph remains acyclic. For the time-resolved fuel flow simulation the entire graph is iteratively processed at each discrete timepoint. The approach allows the MFPE to capture the transient behaviours and dynamic interactions within the fuel flow pathway.

Figure 3-B left side shows backward pass for demand propagation. The graph is traversed in reverse topological order to communicate demand from downstream to upstream nodes based on their respective current

internal state, hence every component requests a certain amount of one or multiple quantities from the respective upstream components.

Figure 3-B right side shows forward pass for supply propagation and flow calculation. The graph is traversed in topological order and for each node the supply is communicated to the downstream nodes, hence every component offers a certain amount of one or multiple quantities to its downstream components.

Concurrently, based on the supply and demand present in the current timestep for all quantity-specific sub-graphs the flow is calculated solving a max-flow problem utilizing the algorithm provided by NetworkX [40]. After the flow calculations for each node its new internal state is evaluated based on the updated flows.

3 Results of the model evaluation

Case study results demonstrate the applicability of the MFPE in assessing and comparing three alternative fuels in five fuel pathways resulting in a total of 21 individually calculated scenarios (Table 2). The MFPE provided KPIs on an hourly time resolution for a simulation period of one year (i.e. 8760h). For each max-flow optimisation, a finite number of iterations was calculated until the dynamic termination criteria were met.

For selected pathways P1 GH2 (Figure 5) and P5 BMeOH (Figure 6) more detailed results are presented to showcase the level of detail the MFPE can provide, including representations of important quantities and

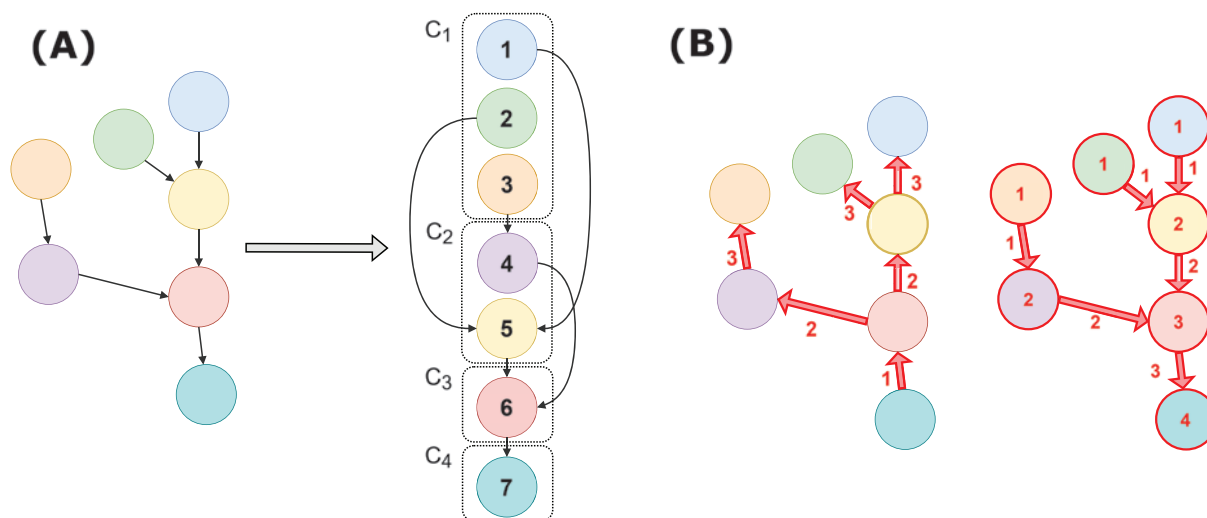


Figure 3: (A) Topologic ordering of a directed acyclic graph, with topologic generations. (B) The schematic shows the backward pass (left) and the forward pass through the graph (right). Diagram from [39] used with permission.

breakdowns of LCOF, sizing of components and feasibility studies for different storage options.

Fuel pathways were built by assembling predefined production, storage, and transport components. Each fuel pathway component was transferred into a Python object with explicitly defined size, storage capacity, and energy supply mode; the simulation time step was set a priori. After the pathway setup and parameter definition, the MFPE ran the time-resolved simulation based on which storage levels, production rates, pipeline throughput, fuelling behaviour and other quantities were returned as pandas DataFrames [41].

The parameter database can be accessed together with the MFPE Python library via the open-source Gitlab repository [38]. This also includes access to all evaluated pathways for the Case Study Port of Rotterdam as Jupyter Notebook tutorials for more in-depth understanding of the calculation path. As the database still needs to be fully validated and parameters such as gas expansion in storage, and large-scale storage cost scaling were not readily available some uncertainty may have been introduced in some of the cost models.

3.1 Fuel pathway modelling results

Figure 4 shows an overview of KPI results for all modelled pathways. W2W efficiency is referenced to PV electricity for RFNBO (P1 GH2, P3 GNH3) and recycled fuels (P4 RNH3) and to biomass input for biofuels (P2 BH2, P5 BMeOH).

Compressed hydrogen shows higher efficiency compared to liquefied hydrogen due to liquefaction losses, while ammonia and methanol pathways generally exhibit better overall energy utilization. Notably, ammonia production via ion exchange from high-N wastewater achieves relatively high W2W efficiency (~38%).

The LCOF for all pathways are calculated by summing up of the component-specific LCOF of the infrastructure, fuel conversion technologies and storage systems. Results indicate that fuel conversion technologies dominate, while infrastructure (e.g. PV, pipelines) contribute to $\leq 5\%$.

Liquefied green hydrogen shows higher costs (65 ± 11 €/MWh propulsion energy) compared to gaseous green hydrogen. Among biofuel pathways, methanol from gasification shows the lowest costs (107–115 €/MWh), while hydrogen pathways are more expensive (227–334 €/MWh). For RFNBO and recycled fuel pathways, hydrogen via PEM is lowest (~169 €/MWh),

followed by ammonia (191–194 €/MWh), with ion exchange at low N-concentrations as most costly.

Looking at the minimum TRL, potential bottlenecks of the biofuel and recycled fuel production technologies can be identified. However, in this overview, no component shows TRL <6, indicating prototype-level validation in relevant environments. Mean TRLs above 8 across all pathways suggest high maturity level, supporting applicability for real-world demonstration despite remaining technological challenges related to scaling.

The amount of PV, biomass, and wastewater necessary for satisfaction of the demand has been evaluated as an additional feasibility check for the pathways. P1 GH2 scenario B requires the largest PV area without grid connection, resulting in an area of >1,000 km² of PV. This is approx. 10-fold larger compared to the world's biggest PV park currently operating in Xinjiang, PRC [42].

For the biofuel P2 BH2 and P5 BMeOH scenario B the biomass feedstock necessary amounts to roughly 30 million t wood per year each – 20 times the annual wood harvests from forests in the Netherlands [43]. P4 RNH3 scenario C would need 48 billion m³ of wastewater to gather the necessary amount of ammonia; in comparison, the Netherlands produce roughly 1.3 billion m³ wastewater per year as per 2020 [44].

3.2 P1 GH2 pathway modelling results

In the detailed simulation the port demand model is integrated with the upstream hydrogen supply system to analyse the interaction between propulsion energy demand, renewable generation, and storage operation. The port component translates annual vessel traffic into a stochastic, time-resolved propulsion energy demand profile, allowing the assessment of demand fulfilment under constrained supply conditions.

Data shown in Figure 5 allows investigation on seasonal effects and its influence on different pathway components for P1 GH2 scenario B. Figure 5-A shows that during the winter months (Nov. - Feb.), reduced PV output results in longer fuelling times and temporary supply limitations. Figure 5-B reflects the storage behaviour, where the salt cavern acts as long-term seasonal storage, gradually depleting during low-generation periods and being rapidly replenished once PV availability increases, while the smaller tank provides short-term balancing with relatively stable operation.

Figure 5-C compares propulsion energy demand at the port with the PV electricity required for hydrogen

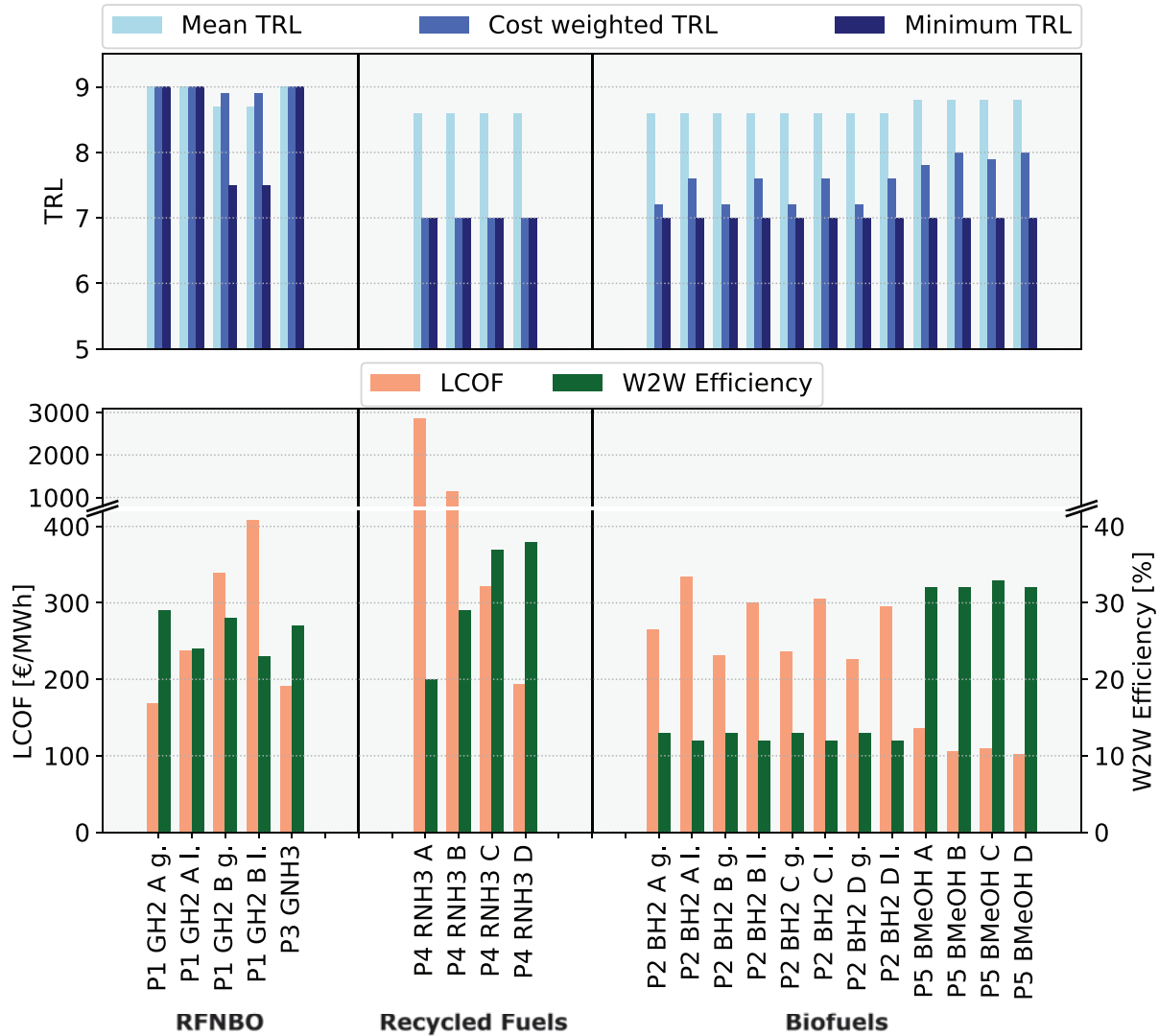


Figure 4: MFPE key performance indicator results including TRL, LCOF and W2W efficiency for the modelled fuel pathways and scenarios. Pathway notation relates to the letters marked in bold in Table 2.

production and highlights the need for increased PEM operation after winter to restore storage levels, which is particularly relevant for system sizing. Figure 5-D reveals LCOF analysis, indicating that overall costs are dominated by the conversion technology (PEM), whereas infrastructure elements such as PV generation, pipelines, and storage contribute comparatively less, underscoring the importance of conversion efficiency and cost in pathway design.

From a land use perspective, PV capacity analysis is highly relevant. By changing the parameters of the defined components (in this case the PV nominal power) for P1 GH2 scenario A its impact on the coverage of

PEM electricity demand, land use, and LCOF can be investigated, under the premise that the demand at the port can be satisfied.

The results in Table 3 indicate diminishing returns with increasing PV size, as doubling the installed capacity leads to only a marginal increase in demand coverage rather than a proportional effect, while land use scales linearly. Furthermore, variations in LCOF are primarily driven by the cost of grid-supplied electricity, whereas the contribution of increased PV capacity to overall cost changes remains comparatively limited.

If P1 GH2 scenario A were operated in an island configuration (i.e. without grid connection) on the other

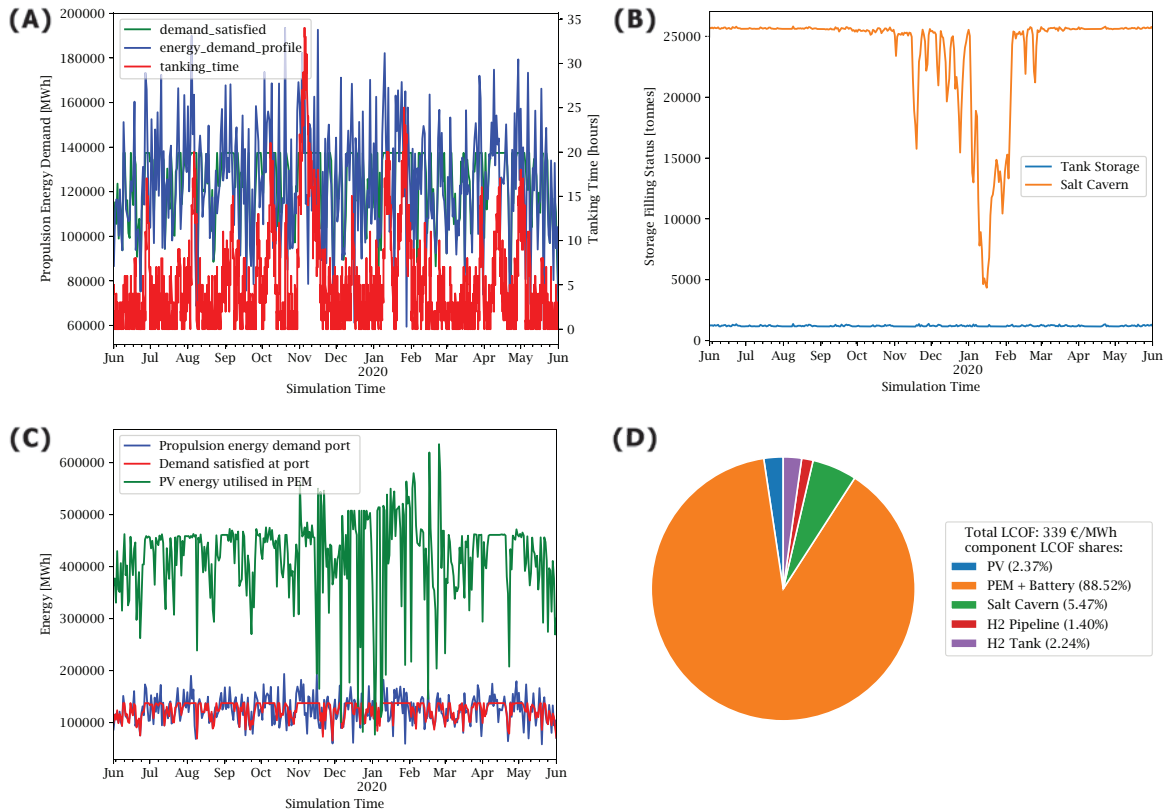


Figure 5: Results for P1 GH2 scenario B - (A) Demand profiles and tanking time at the port; (B) Storage filling status of salt cavern and tank; (C) Demand profiles at port in comparison with the PV energy utilised in PEM production; (D) LCOF with component shares.

hand, the question arises whether battery storage or hydrogen storage makes more sense for the needed buffering, when PV generation is not available. This can be answered through a feasibility study like the one presented in Table 4 by adjusting various component parameters. Port fuel demand was set as prerequisite, thus the sizes of the components have been defined accordingly.

The results show the cost-effectiveness of increasing hydrogen storage over battery storage, even though a larger electrolyser is required in this case. This is more pronounced in Conf. 7 without any battery storage. Sensitivity evaluations reflect the suitability of hydrogen storage for long-term balancing, whereas battery systems become less economical at larger scales and have a negative effect on the ship fuelling time at the port.

Table 3: Results of study on varying PV capacity (P1 GH2 scenario A).

	PV nominal power [MW]		
	80,000	160,000	320,000
Coverage of PEM consumption through PV [%]	33.0	38.2	42.4
Land use [km ²]	400	800	1,600
LCOF [€/MWh]	178	169	161
Part of PV in LCOF [€/MWh]	2.5	2.9	3.3
Part of grid-supplied electricity in LCOF [€/MWh]	128.7	118.6	110.6
Part of PEM in LCOF [€/MWh]	27.7	27.6	27.6

Table 4: Comparison of feasibility of storing electricity vs hydrogen for P1 GH2 scenario A in island operation.

	Conf. 1	Conf. 2	Conf. 3	Conf. 4	Conf. 5	Conf. 6	Conf. 7
PV nominal power [MW]	640,000	640,000	640,000	640,000	640,000	640,000	640,000
Battery capacity [MWh]	733,200	408,900	366,600	274,950	188,000	141,000	0
PEM [t/h output]	390	580	780	1,170	2,000	3,000	3,000
Tank storages [t] / max inflow [t/h]	1,170/390	1,740/580	2,340/780	3,510/1,170	6,000/2,000	9,000/3,000	9,000/3,000
Pipeline throughput [t/h]	390	580	780	1,170	2,000	3,000	3,000
LCOF [€/MWh]	876	528	497	425	393	419	261
Max. Tanking time [h]	70	100	85	70	42	30	40

3.3 P5 BMeOH pathway modelling results

For biofuels, the P5 BMeOH scenario A shows the following detailed results. Figure 6- A compares biomass and PV input energy with port demand providing an indication of overall pathway efficiency (well-to-wake) and supports system sizing by highlighting conversion losses. Figure 6-B shows LCOF analysis, where biomass gasification (~62%) is the dominant cost driver followed by PEM (~34%), while infrastructure contributions are little, emphasizing the importance of conversion technologies for both efficiency and cost. However, transportation and storage of the biomass feedstock has not been considered here.

4 Discussion of key findings and fuel pathway applications

The presented discussion focuses on fuel pathway comparison, simulation tool exploration and valida-

tion, discussion of the MFPE’s potentials and limitations and the transferability of the MFPE framework to other pathway problems and/or other industries.

4.1 Fuel pathway comparison

For all fuel pathways, system boundary conditions prerequisites depend largely on the port infrastructure. While many components could be covered, biomass transport and other forms of electricity generation (except PV) are currently not included and need to be implemented at a later state. Upscaling ship fleet sizes to large container vessels >10MW propulsion energy strongly influences capacity requirements on port-based fuel storage. For artificial storage systems this may be less of an issue, however for geological features such as salt caverns, this is highly specific on the geographical availability.

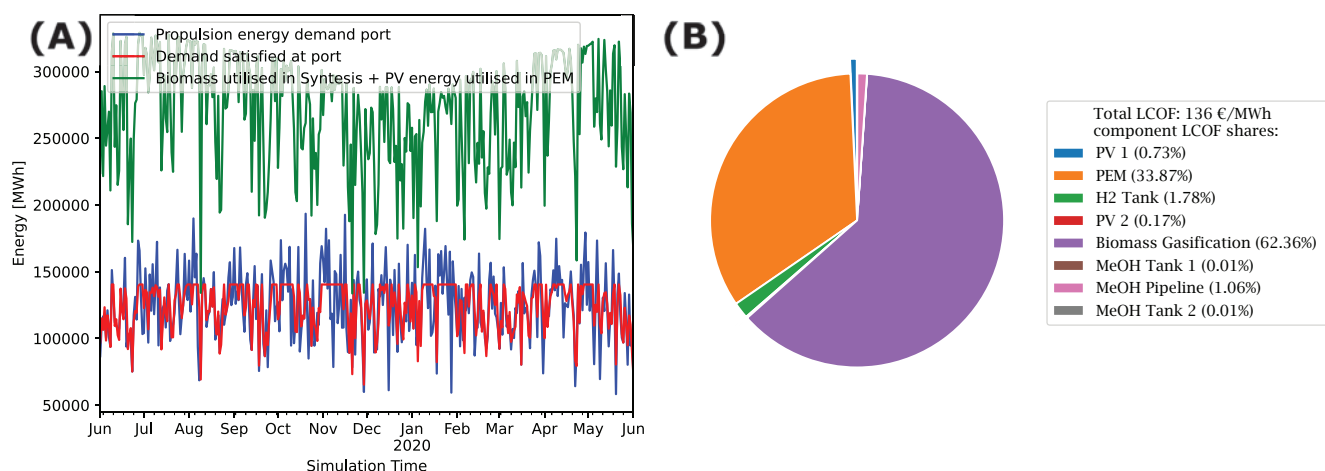


Figure 6: Results for P5 BMeOH scenario A - (A) Demand profiles at port in comparison with the PV energy utilised in PEM production; (B) LCOF with component shares.

The modelled results show that the fuel pathway selection and fuel carrier are strongly linked to both cost and well-to-wake performance. Hydrogen (liq.) emerges as comparatively expensive and relatively inefficient, while hydrogen derivatives such as MeOH and NH₃ can offer more favourable cost–efficiency trade-offs when matched with suitable production and port infrastructure.

Across all fuel pathways, the cost structure analysis reveals that infrastructure elements (e.g. pipeline, PV) have relatively little cost contribution to the overall LCOF (often $\leq 5\%$), indicating that transport and renewable electricity can be scaled with little impact on total costs. However, fuel production largely dominates the total fuel pathway costs ranging from 62 % for PEM electrolysis in P1 GH2 scenario A up to ~100 % in P4 RNH₃ scenario A and B.

These results suggest that strategic investments in highly efficient fuel conversion technologies and process integration will have a much higher impact compared to infrastructure investments.

It is also evident, that land and feedstock availability can be a decisive bottleneck for energy transition of the maritime sector if efficiencies do not increase significantly. However, here also other options should be modelled including offshore wind or offshore PV and other fuel conversion technologies. Storage facilities, and non-PV renewable electricity generation close to ports are enablers but could present major economic bottlenecks at port demand scale.

Therefore, port-centred fuel hubs, combined with carefully designed pathways, may offer a beneficial option. Here harbour authorities, policymakers and vessel producers may have viable entry-points in prioritising sustainable alternative fuel pathways which are economically viable and scalable for slow transitioning of maritime defossilisation.

4.2 Simulation tool validation

There are different approaches to model validation, as explained in [45] for the EnergyPLAN model, based on (i) replication and calibration, (ii) comparison and (iii) open source as validation. However, it is essential to take into account that the validity and applicability of a model is always limited in terms of space, time, and boundary conditions [46].

For the MFPE, the comparability of the selected RFNBO, recycled fuel and biofuel pathways remains difficult due to the fundamental differences in system

boundary conditions, input streams and individual component models and needs harmonization, which requires model calibration data. However, availability of such datasets especially at the modelled supply and demand scale is lacking, as cost and performance data is hard to come by from port operators, energy companies or official authorities.

Furthermore, feedstock transport for biofuels is currently neglected and biomass pathways are calculated based on their caloric energy value, without energy need for transportation.

The MFPE modelling framework is robust and infrastructure scaling has been implemented thoughtfully. While parameterization for transient and cost-scaling data remains a limiting factor, further improvements should be made to refine and harmonize this with more literature sources or verified databases for the desired model application. The MFPE was designed for sustainable alternative fuel pathways and current component sizing goes beyond available datasets.

Validation of the availability and characteristics of input streams must be critically assessed for each application. It is therefore crucial that physically valid system configurations are defined based on sound technical understanding and expert knowledge to ensure that the resulting model outputs remain physically consistent and meaningful either for relative or when fully validated for absolute comparisons.

Therefore, harbour operators and fuel providers should be invited in testing the software and evaluating the results in the context of their operational experience. This may provide valuable practical feedback and help assess the plausibility of individual components and related model output.

Additionally, further validation may also involve comparison of MFPE results against existing software tools with similar modelling capabilities. As there are currently no similar tools available, a combination of established modelling tools could be used to cross-check MFPE's results at different levels of detail. It may be applicable to apply TEA tools for cost comparison, in combination with Aspen Plus [21] for validation of component-level thermodynamic performance and process efficiencies. Further GREET [24] could be applied for life-cycle assessment references for verifying MFPE's energy and resource indicators.

The MFPE library was also made available open source as a Gitlab repository including all utilized data,

modelled fuel pathways, and parameters to establish a user and developer community which may further thrive and implement improvements which is highly desired by the authors.

4.3 MFPE potentials and limitations

The modular plug-and-play structure of the MFPE allows the flexible combination of components to customize pathway design and enables extension with new components and KPIs, which is invited through open collaboration through the open-source availability of the MFPE. As such, the framework supports both adaptability and transferability, ensuring that it can be effectively applied to a wide range of use cases and future developments in renewable fuel systems.

Through the time-resolved simulation dynamic system behaviour can be explored, capturing infrastructure/sizing bottlenecks and seasonal effects, while KPIs enable a quantitative comparison between alternative fuel pathways.

However, this comes with high computational complexity, as multiple max-flow problems must be solved at every simulation time step. Automated component sizing is therefore challenging, particularly for large design spaces or long simulation periods.

Additionally, the quality of results strongly depends on the completeness and reliability of the parameter database as discussed above. Limited availability of comparable datasets especially for upscaling of component models and full-system benchmarks constrains validation, while the exclusion of most site-specific factors—such as terrain or climate—reduces generalisability.

It is also important to consider that the definition of meaningful system boundaries as well as the interpretation of the results requires expert knowledge to conduct structured scenario analyses and to derive well-founded insights from the simulation results.

4.4 Transferability to other industries

Although the MFPE framework, the presented fuel pathways, and the concept for a multi-fuel SOFC were primarily developed and applied for the maritime sector, the overall modelling framework and its modularity make a modification attractive also for other sectors and problems.

The characteristics of time-resolved modelling, fuel demand and supply profiles, and focus on alternative fuels may be easily transferable to scenarios related to

energy supply for inland shipping, industrial hubs or even railway.

For inland shipping, fuel demand and supply are in an achievable scale as presented in the results above. If fuel cells for propulsion will be applied is to be debated, however any other propulsion type can be integrated in the MFPE.

For industrial hubs, most relevant sectors for SOFCs are food and beverage, paper, or chemical processing which have high electric and thermal demands in achievable temperature levels [47]. Techno-economic analyses confirm the competitiveness of SOFC systems under realistic industrial demand profiles, especially when operated with low-carbon fuels such as hydrogen or biogas [48]. This study examines the feasibility of using hydrogen as a clean energy source for residential consumers in the UK through a low-carbon energy hub. Two cases were compared: a solid oxide fuel cell (SOFC).

For railway, especially highly frequented railway lines are electrified, while remote and low-frequented lines could be equipped with multi-fuel SOFCs instead of diesel engines to reduce carbon emissions. The challenges include load variability and dynamic response as well as fuel flexibility in the railway context [49], the latter being addressed in [50] which investigates ammonia and hydrogen in hybrid freight train concepts.

5 Conclusion and outlook

The developed multi-fuel pathway explorer (MFPE) allows modelling of entire fuel pathways from feedstock until utilization in SOFC for the maritime sector. Pathway modelling includes components covering electricity generation, fuel conversion, storage, and distribution aspects for application of an SOFC.

The KPI-based evaluation provides TRL, LCOF and W2W efficiency, including time-resolved demand and supply profiles over all components allowing for a comprehensive assessment of technical performance and comparison. The high time resolution of one hour can be exploited for optimization on component-level (e.g. sizing of fuelling and storage systems), which is impossible when only using annual averages. This enables the identification of process bottlenecks and interdependencies.

The current development state of the MFPE was tested under set conditions and is currently functional and applicable for exploratory analyses of the proposed

fuel pathways. Nevertheless, further validation and verification, for instance through collaboration with harbour operators and industry stakeholders, to ensure practical accuracy and reliability is recommended. The model structure allows for broad applicability to additional use cases within and beyond the maritime sector, if component parameters and system boundaries are adapted to reflect the characteristics of the respective industrial, transport, or energy contexts.

MFPE users and developers are permitted to freely build and implement their own fuel pathways, scenarios, and case studies. The user is guided by specifically designed Jupyter Notebook tutorials which allow rapid screening of high potential pathways and easy application use. However, currently certain limitations remain, particularly regarding simplifications in system dynamics and the need for full model validation. Due to the open-source licence, developers, experts, and any users are highly invited to further develop the MFPE in areas of the indicated limitations and to verify their modelling results themselves.

The authors suggest that further MFPE application and development should focus on the validation and verification of the model outputs, the extension of component library and parameter database, and the refinement of parameterization and data integration methods.

Since recently an open database for LCA and sustainability data was released through the openLCA Nexus [51], the aspects of GHG or other environmentally relevant parameters can now be included in the open-source MFPE library as well. The combination with LCA databases will strengthen the MFPE's robustness and enhance its role as a decision-support tool for the rapid pre-selection of sustainable alternative fuel pathways for further in-depth investigation.

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