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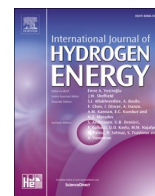
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Sustainability assessment of methanol steam reforming reactors for shipboard coupling with PEM fuel cells

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ABSTRACT

Onboard methanol steam reforming (MSR) coupled with proton exchange membrane fuel cells (PEMFCs) is investigated as a pathway for maritime decarbonization. Joule heating, flue-gas heating, and condensing-steam heating of multitubular fixed-bed MSR reactors are compared using steady-state one-dimensional models and technological, economic, environmental, and safety indicators. Selected configurations achieved weighted-average methanol conversions higher than 99%. Joule heating produced inlet cold spots of 442–445 K, whereas condensing steam maintained nearly uniform temperatures of 477–478 K. Within the investigated candidate set, normalized aggregated sustainability indicators ranged from 0.64 to 0.88 for Joule heating, 0.87–0.96 for flue-gas heating, and 0.997–0.999 for condensing steam. Condensing-steam heating attained the highest aggregate ranking across the examined decision-making perspectives and aggregation procedures. These relative indicators are not absolute sustainability levels, and the ranking remains conditional on the investigated steady-state design space, system boundaries, model assumptions, and economic and emission factors.

Nomenclature

A	Surface area	$k_{m,i}$	I-th component mass transfer coefficient
a_{part}	Catalyst particle volume-specific surface	K_s	Site-specific adsorption constant
C_i	I-th component concentration	K_r^{eq}	Reaction's equilibrium constant
$C_{i,surf}$	I-th component concentration at catalyst external surface	KPI	Key performance indicator
C_{lim}	Limiting reactant concentration	KPI_{add}	Aggregated additive KPI
$\hat{C}_p$	Mixture mass-specific heat capacity	KPI_{geo}	Aggregated geometric KPI
CAPEX	capital expenditures	L_{tot}	Total tube length
$CO_{2,eq}$	Equivalent carbon dioxide emission	LNG	Liquefied natural gas

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D	Tube internal diameter	$\dot{m}_{CO_{2,eq}}^{(1)}$	Direct process GHG emission rate
d_{part}	Catalyst particle diameter	$\dot{m}_{CO_{2,eq}}^{(2)}$	Electricity-associated indirect GHG emission rate
d_{eq}	Equivalent hydraulic diameter	$\dot{m}_{CO_{2,eq,k}}^{(out)}$	Equivalent GHG emission rate associated with the k-th process component
d_{ext}	Tube outer diameter	$\dot{m}_k^{(out)}$	Mass flow rate of the k-th process component
DF&EI	Dynamic Fire and Explosion Index	$\dot{m}_{steam}$	Steam mass flow rate
Eco	Economic indicator	MSR	Methanol steam reforming
EF_k	Emission factor	MD	Methanol decomposition
Env	Environmental indicator	n	Economic lifespan of the ship power system
F_m	Material factors	$\dot{n}_{CH_3OH,in}$	Inlet methanol molar flow rate

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F&EI	Fire and Explosion Index	N_b	Number of baffles
GHG	Greenhouse gas	N_{comp}	Total number of components
GWP	Global warming potential	N_r	Total number of reactions
h_T	Heat transfer coefficient	N_t	Total number of tubes
I	Electrical current per tube	OPEX	Operating expenditures
IMO	International Maritime Organization	$\mathbb{P}$	Power demand of the process
k_{app}	Apparent kinetic constant	p_i	Partial pressure of the i -th species
k_k	Reaction kinetic constant	t_w	Tube-wall thickness
P_{tubes}	Tube-side pressure	T_{wall}	Tube-wall temperature
PEMFC	Proton exchange membrane fuel cells	$Tech$	Technological indicator
r	Discount rate	U	Overall heat transfer coefficient
$\mathcal{R}_r$	Reaction rate	v_z	Superficial axial velocity
S_{BET}	BET surface area	WGS	Water-gas shift
s_i	i -th sector and related factor	z	Dimensional axial coordinate
Safe	Safety indicator	$\Delta \tilde{H}_{r,298K}$	Molar reaction enthalpy at 298 K
shell	Shell side index	$\Delta \tilde{H}_{vap}$	Specific latent heat of water vaporization
span	Sector's span	ΔT_d	Deactivation temperature distance
T	Mixture temperature	ε_{bed}	Bed void fraction
T_d	Catalyst deactivation temperature	η	Catalyst effectiveness factor
$T_{shell}^{eq}(P_{shell})$	Shell-side equilibrium temperature	μ	Fluid viscosity
T_{min}	Minimum recorded temperature	$\nu_{i,r}$	i -th component stoichiometric index in the r -th reaction
T_{opt}	Optimal operating temperature	ρ	Mixture density
T_{score}	Temperature score factor	ρ_{bulk}	Catalyst bulk density
T_{shell}	Shell-side temperature	$\rho_{e,wall}$	Wall electrical resistivity
T_{surf}	Temperature at catalyst external surface		

1. Introduction

The maritime sector is undergoing a major transition driven by increasingly stringent environmental regulations and the need to reduce greenhouse-gas (GHG) emissions associated with global shipping activities [1]. Maritime transport currently accounts for approximately 3% of global CO₂ emissions, and this contribution is expected to increase with the continuous growth of international trade [2]. In response, the International Maritime Organization (IMO) has established ambitious targets aimed at substantially reducing GHG emissions from shipping by 2050 [3]. Achieving these objectives requires the development of alternative onboard power-generation systems capable of combining high efficiency, operational flexibility, and reliability under highly dynamic shipboard operating conditions [4]. Several pathways are currently being explored for maritime decarbonization, including direct electrification, low-carbon fuels, and hydrogen-based energy systems [5, 6]. Battery-electric propulsion provides high efficiency and zero-emission operation at the point of use, although its applicability remains mainly limited to short-range vessels due to battery energy density and weight constraints [7]. Alternative fuels such as LNG, ammonia, and methanol have therefore attracted increasing interest for medium- and long-range applications [8,9].

Among these solutions, hydrogen-based power systems coupled with proton exchange membrane fuel cells (PEMFCs) are considered a promising solution for low-emission maritime propulsion and auxiliary power generation due to their high electrical efficiency, rapid dynamic response, and compatibility with variable shipboard power demand [10–12]. However, the widespread adoption of hydrogen onboard ships is still limited by storage-related challenges, since cryogenic or high-pressure hydrogen tanks introduce significant penalties in terms of volume, weight, and safety management [13]. Consequently, increasing

attention has been devoted to hydrogen carriers enabling onboard hydrogen production [14,15].

Methanol has emerged as one of the most attractive hydrogen carriers for maritime applications due to its high volumetric energy density, liquid-phase storage under ambient conditions, compatibility with existing bunkering infrastructure, and potential production from renewable feedstocks and captured CO₂ [12,16]. In this context, methanol steam reforming (MSR) coupled with proton exchange membrane fuel cells (PEMFCs) represents a promising solution for onboard hydrogen-based power generation in maritime applications [17]. In these systems, methanol is converted into a hydrogen-rich stream through a strongly endothermic catalytic process, whose thermal management plays a critical role in reactor performance and system integration, followed by hydrogen purification to satisfy PEMFC fuel-quality requirements and electrochemical power conversion [18]. Despite its potential, the implementation of methanol steam reforming reactors onboard ships introduces challenges that substantially differ from those encountered in stationary applications [19]. Shipboard systems must operate under variable power demand while satisfying strict constraints in terms of compactness, weight, operational flexibility, and safety [20].

Recent developments in other strongly endothermic reforming processes highlight the close interplay between reaction conditions, thermal management, and catalyst architecture. In methane dry reforming, the controlled structural evolution of Ni-Ce bimetallic alloys supported on Al₂O₃ has shown that optimized Ce incorporation can improve active-metal reducibility and dispersion, generate oxygen vacancies, enhance reactant adsorption and activation, and suppress carbon accumulation during prolonged operation [21]. Advanced multi-interface architectures have also been proposed, including the dynamic anchoring of Co_{0.1}Ce_{0.1}Ni_{0.8} trimetallic alloys on Ti₃C₂ MXene/g-C₃N₄ composites. By combining tunable alloy active sites with enhanced interfacial energy and charge transport, these materials enable efficient conversion under milder photothermal conditions while improving resistance to carbon deposition [22]. Furthermore, high-entropy catalysts based on multi-component Co-Ni-La-Ca-Ce systems exploit compositional disorder, lattice distortion, sluggish diffusion, and synergistic effects to broaden the operating-temperature window, regulate product selectivity, and mitigate catalyst sintering and carbon formation [23].

Although methane dry reforming and MSR involve different reaction mechanisms, catalyst formulations, and operating temperatures, these studies suggest potentially transferable catalyst-design principles for the future optimization of shipboard MSR catalysts. In particular, promoter-assisted defect engineering, multimetallic active-site modulation, and the development of thermally robust catalyst-support interfaces could be adapted to MSR catalysts to enhance low-temperature activity, limit CO formation, and improve resistance to deactivation. Such catalyst-level strategies could complement reactor-level thermal management by extending the effective operating window and supporting stable reformer performance under compact and demanding marine conditions.

In this context, heat supply becomes a critical aspect of reactor design due to the strongly endothermic nature of the methanol steam reforming process [24]. Insufficient heat transfer may lead to inlet cold spots, reduced methanol conversion, and catalyst deactivation, whereas excessive heating can result in thermal stresses, overheating, and reduced process efficiency. Different heating strategies can be adopted to sustain the reforming reaction, including direct electrification through Joule-heated walls [25], indirect heating by flue-gas streams [26], and condensing-steam-based heating [27]. These approaches exhibit substantially different thermal behaviour, controllability, utility requirements, and integration complexity under shipboard operating conditions. The selection of the heating strategy becomes a key aspect in the design and operation of onboard MSR/PEMFC systems, particularly under fluctuating auxiliary and propulsion power demand [28,29].

Previous research relevant to the present work can be grouped into four principal areas. First, studies on MSR catalysts and reactor

development have primarily investigated reaction kinetics, catalyst performance, methanol conversion, selectivity, and conventional or membrane-reactor architectures [30,31]. Second, recent investigations have addressed individual heat-supply concepts, including Joule-heated catalytic microreactors [32], engine-exhaust-heated packed-bed reactors [33], and reformers exploiting the condensation enthalpy of water vapour [27]. These studies provide important information on the individual technologies but do not compare the different heating mechanisms within a common reactor-design framework, kinetic formulation, hydrogen-production requirement, design constraints, and system boundary. Third, shipboard reforming studies have examined oxidative methanol reforming integrated with fuel cells [34], methane- and methanol-based fuel-processing systems coupled with HT-PEMFCs and carbon capture [35], and the transient response of shipboard MSR reactors [36]. However, their primary objectives concern process integration, fuel and carbon-management strategies, or reactor dynamics rather than the system-level consequences of alternative MSR heat-supply strategies. Finally, existing multicriteria assessments have compared complete maritime power systems [37] or proposed general KPI-based methodologies for sustainable reactor design [38], without resolving how the reactor-heating mechanism propagates through reactor thermal behaviour, equipment design, utility integration, and overall sustainability in a shipboard MSR/PEMFC system.

Complementary system-level studies further demonstrate the importance of evaluating the reformer together with hydrogen purification, heat recovery, the fuel cell, and balance-of-plant components. Energy–exergy analyses of integrated small-scale steam-methane-reforming/LT-PEMFC systems and kerosene-reforming PEMFC cogeneration systems have shown that system efficiency and irreversibilities depend strongly on reformer operating conditions, heat recovery, and fuel-cell operation [39,40]. More recent studies have extended this perspective to variable-power multi-fuel reforming systems, including methanol, through combined forward–backward thermodynamic analysis [41], integrated feasibility, environmental, and economic assessments for reliable off-grid power generation [42], and kW-scale experimental demonstrations including comparisons among electrical heating, combustion heating, and heat-recovery architectures [43]. Collectively, these studies confirm that reformer performance should be assessed within the broader energy-conversion system and that heating and heat-integration choices can influence efficiency, emissions, and economic performance. However, they do not provide a controlled comparison of alternative heating mechanisms for shipboard MSR reactors within a common reactor-design, operating, and sustainability-assessment framework.

Against this background, the methodological novelty of the present work does not reside in the isolated use of a one-dimensional reactor model or a multicriteria assessment procedure. Rather, it lies in integrating reactor design, thermal analysis, ship-level energy integration, and multidomain sustainability assessment within a controlled comparative framework in which Joule, flue-gas, and condensing-steam heating are evaluated using the same reaction kinetics, catalyst properties, feed conditions, hydrogen-production targets, design constraints, and system boundaries. This common basis allows the influence of the heat-supply mechanism to be examined on a controlled comparative basis while minimising differences arising from catalyst formulation, reactor duty, scale, or modelling assumptions. The framework further extends previous KPI-based reactor-design methodologies by incorporating multiple time-weighted steady-state operating regimes representative of auxiliary and propulsion demand, maritime redundancy requirements, reactor-level thermal behaviour, and ship-level heat and power integration.

More specifically, the present study provides four main advances: (i) a consistent design and steady-state off-design comparison of multitubular Joule-, flue-gas-, and condensing-steam-heated MSR reactors; (ii) an explicit connection between the spatial relationship of reaction heat demand and heat supply and the resulting axial temperature

profiles, cold spots, overheating, catalyst utilisation, reactor geometry, pressure drop, and utility requirements; (iii) an integrated technological, economic, environmental, and safety assessment over representative time-weighted auxiliary and propulsion operating regimes; and (iv) evaluation of the stability of the resulting technology ranking across four decision-making perspectives and both additive and geometrical aggregation procedures. The contribution is therefore both methodological and practical: the proposed framework provides a reproducible comparative basis to inform heating-strategy selection within integrated shipboard MSR/PEMFC systems and assesses how the choice of heat-supply mechanism affects reactor thermal behaviour, system-level energy integration, and sustainability performance.

2. Methodology

The methodological framework adopted in this work combines process modelling, reactor design, and sustainability assessment to evaluate alternative heating strategies for methanol steam reforming integrated with PEM fuel-cell systems in maritime applications. Electrified, flue-gas-heated, and condensing-steam-heated reactor configurations are comparatively assessed under representative shipboard operating conditions through reactor-level and system-level analyses, coupled with a KPI-based sustainability evaluation.

2.1. Definition of the analysed system

The present study investigates the integration of methanol steam reforming (MSR) reactors with proton exchange membrane fuel cells (PEMFCs) for onboard hydrogen-based power generation in maritime applications. To enable a consistent comparison among alternative reactor-heating strategies, a simplified yet representative process configuration is adopted, including the main units involved in reactant conditioning, hydrogen production and purification, thermal integration, and electrochemical power conversion. The reference process flow scheme considered throughout the analysis is shown in Fig. 1.

Referring to Fig. 1, methanol and water are supplied to dedicated conditioning lines, where they are pressurised, pre-heated, vaporized, and superheated before entering a multitubular fixed-bed reformer. Within the reactor, methanol steam reforming converts the reactant mixture into a hydrogen-rich stream through a catalytic reaction network. The reformat is subsequently purified through a palladium-based membrane unit to satisfy the hydrogen-purity requirements of the PEMFC system [44]. In the present work, the membrane is represented by a fixed hydrogen recovery factor of 80%, accounting for separation losses and process inefficiencies [45]. The purified hydrogen is supplied to the PEMFC unit for electrochemical power generation, whereas the membrane retentate, containing residual combustible species and reaction by-products, is processed in a catalytic burner to recover additional chemical energy. The recovered thermal energy is partially reused within the process to support reactant conditioning and improve overall thermal integration.

The selected value is intended as a representative design assumption rather than an optimized or universally achievable membrane performance. Experimental studies of methanol steam reforming with dense Pd-based membranes have reported hydrogen recoveries of approximately 74–85%, including values close to 80% with very high hydrogen selectivity [46,47]. The same recovery factor is applied to all configurations to provide a consistent hydrogen-delivery basis. However, sensitivity to membrane recovery was not assessed, and the adopted value should therefore be regarded as a fixed modelling assumption.

Three alternative reactor-heating strategies are comparatively investigated: direct electrification through Joule-heated reactor walls (A), indirect heating by hot flue-gas streams (B), and condensing-steam heating (C). These configurations differ in their heat-transfer mechanisms, utility requirements, and integration within the onboard energy system. The investigated system is evaluated under representative

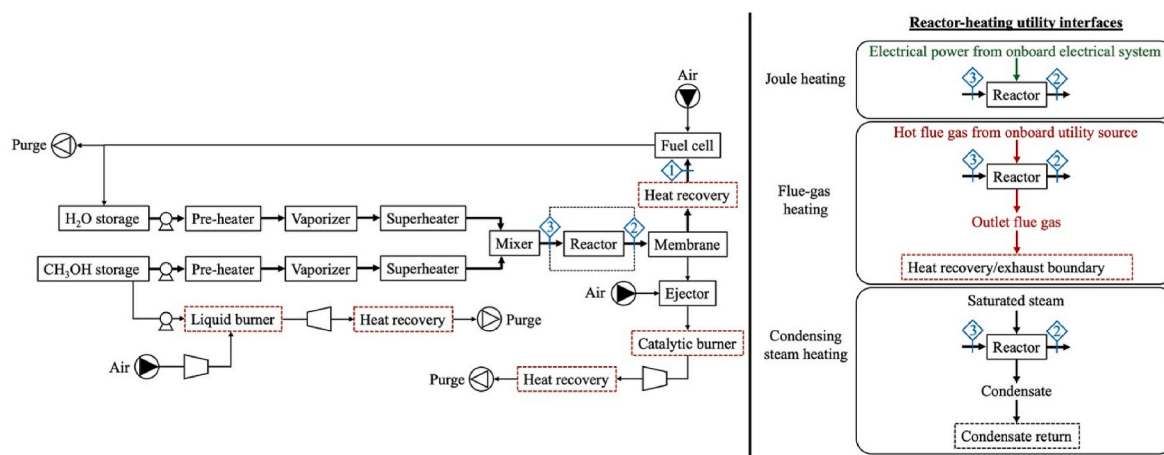


Fig. 1. Reference process-flow scheme and reactor-heating utility interfaces adopted in the analysis. Dashed boxes indicate heat-recovery and auxiliary-heating functions included in the system-level energy balance. The right-hand inset distinguishes the Joule-, flue-gas-, and condensing-steam-heating interfaces and their corresponding utility boundaries. External utility-generation, conditioning, distribution, and return networks are not explicitly modelled. Main process-stream tags are shown in blue.

shipboard operating conditions covering both auxiliary and propulsion power-generation scenarios. Since maritime power demand is inherently variable, multiple discrete steady-state operating points associated with different hydrogen-production requirements are considered to assess reactor performance across the ship load profile. Transitions between these operating points are not simulated. System-level redundancy requirements typical of maritime applications are explicitly incorporated into the analysis. Propulsion power is assumed to be provided by two identical reactors operating in parallel to ensure operational continuity and minimum propulsion capability in the event of the failure of a single unit, in line with regulations [48] and common practices [49]. Accordingly, the design flow rates for propulsion applications are equally distributed between the two reactor units, whereas auxiliary systems are modelled with a single operating reactor supported by an identical standby unit and are therefore designed based on the full calculated demand.

Fig. 1 defines the process and utility boundaries adopted in the present assessment and, through the reactor-heating inset, distinguishes the interfaces associated with the three heating configurations. It is not intended to represent a detailed engineering design of the complete onboard utility networks. For Joule heating, electrical power is supplied directly to the reactor walls. For flue-gas heating, hot gas enters the reactor shell side under the prescribed inlet conditions, transfers sensible heat to the reacting tubes, and exits at the downstream heat-recovery/exhaust boundary. For condensing-steam heating, saturated steam enters the shell side at the prescribed pressure, releases latent heat through condensation, and exits as condensate at the condensate-return boundary. Utility generation, conditioning, distribution, pressure control, and return networks depend on the vessel-specific energy architecture and are therefore not explicitly designed or simulated. Their influence on the comparison is represented through the prescribed reactor boundary conditions and the global energy and utility balances included in the sustainability assessment. The scheme should therefore be interpreted as a functional representation of the system and heating interfaces relevant to the present analysis rather than as a detailed shipboard plant layout.

To satisfy residual thermal requirements associated with reactant conditioning and process heat duties not covered by recovered energy, an auxiliary methanol-fuelled heating system is included. Air supply to the catalytic burner is provided through an ejector-based configuration, thereby avoiding the need for dedicated compression systems. In both energy-recovery sections, only sensible heat recovery is considered, and the exhaust temperature is fixed at 383 K to prevent condensation and associated corrosion phenomena. Electrical consumption is associated

with pumps and compressors, whereas electricity generation is obtained from turbine-expanders with a mechanical-to-electrical conversion efficiency of 85%.

The system-level calculations are deterministic process models formulated from material and energy balances and literature-based component relations. They use the reactor outputs together with the specified hydrogen-recovery factors, component efficiencies, and utility assumptions. Material- and energy-balance closure was checked during model development for the reported calculations, although the corresponding residual values were not retained for quantitative reporting. The individual system-level component models were not independently experimentally validated in the present study.

2.1.1. Ship operating regimes and hydrogen demand

Proton exchange membrane fuel cells (PEMFCs) rated at 225 kW are adopted as reference technology [50], and the corresponding hydrogen consumption is estimated from manufacturer operating data while accounting for performance degradation at end-of-life conditions [51] and the yearly operational load profile of an 87 m yacht provided by Feadship Royal Dutch Shipyards. The corresponding methanol feed rates required for onboard hydrogen production through methanol steam reforming are determined. Multiple operating regimes associated with different power-demand levels and operating time shares are considered to capture the variable-load nature of shipboard operation. To reduce the complexity of the analysis while preserving representative operating conditions, regimes characterized by time shares lower than 1% are excluded, assuming that short-duration peak loads can be managed through auxiliary energy-storage systems (Table 1).

2.1.2. Process operating conditions

The operating conditions of the methanol steam reforming process are selected to ensure compatibility with PEMFC requirements while ensuring technically feasible steady-state reactor performance at the investigated shipboard operating points. The reactor inlet temperature is fixed at 523 K, representing a compromise between sufficient catalytic activity and catalyst thermal stability for Cu-based reforming catalysts (CuO/ZnO/Al₂O₃ pellets) [52]. The operating pressure is 5 bar to facilitate the integrated hydrogen purification units and PEMFC technologies [53,54]. The inlet steam-to-methanol molar ratio is fixed at 1.5 to provide a balance between carbon-monoxide suppression, catalyst stability, and the reduction of excessive energy consumption associated with water vaporization [55–57]. The methanol feed rate varies according to the hydrogen demand associated with the different ship operating regimes described in Table 1. For each investigated

Table 1

Hydrogen and methanol flow rates for the specified operating time shares in auxiliary and propulsion power systems.

Power system	Operational time share [%]	H ₂ flow to the fuel cell [kmol/h]	H ₂ flow to the membrane [kmol/h]	Methanol flow to the reactor [kmol/h]
		Stream 1	Stream 2	Stream 3
Auxiliary power	9	3.42	4.25	1.42
	26	4.54	5.65	1.88
	20	5.74	7.13	2.38
	13	7.00	8.68	2.90
	3	8.39	10.40	3.47
Propulsion power	2	9.96	12.35	4.12
	2	43.60	54.07	18.02
	7	48.19	59.65	19.89
	7	52.60	65.23	21.74
	4	57.01	70.70	23.57
	5	61.94	76.79	25.60
	2	66.75	82.76	27.59

configuration, reactor operation is evaluated under multiple load conditions while ensuring a minimum methanol conversion of 99% under nominal operating conditions.

2.2. Reactor modelling

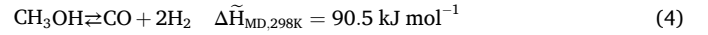
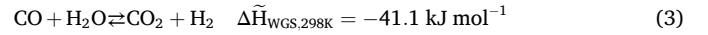
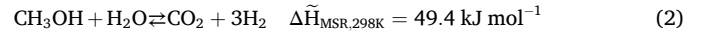
In the present study, methanol steam reforming is carried out in a multitubular fixed-bed shell-and-tube reactor. The multitubular configuration allows the catalytic reaction to occur inside catalyst-packed tubes, while heat is supplied from the shell side through the selected heating medium [24,44,58]. The reactor is modelled as a one-dimensional plug-flow system accounting for mass, energy, and momentum balances along the axial coordinate, while radial gradients in the gas phase are neglected. Thermodynamic and transport properties are evaluated as temperature- and pressure-dependent quantities to ensure consistency among kinetic, thermal, and fluid-dynamic calculations. Furthermore, the reactor geometry determined during the design stage is maintained unchanged during off-design simulations, while only the operating conditions are varied to reproduce the different ship operating regimes. Pressure drops are evaluated through momentum balances accounting for frictional effects across the catalytic section, following the Ergun equation. Energy balances include reaction enthalpy contributions, convective heat transport, and heat exchange between the reacting mixture and the external heating medium. To account for intra-particle transport limitations without explicitly resolving detailed pore-scale phenomena, diffusion effects within the catalyst pellets are incorporated through an effectiveness-factor approach. This formulation enables the representation of mass-transfer limitations while maintaining computational efficiency suitable for the extensive parametric analysis performed in the present study.

The effectiveness factor, η_r , in Equation (1) accounts exclusively for diffusion–reaction limitations within individual catalyst pellets and does not represent reactor-scale radial transport. Radial temperature and concentration gradients across the packed bed are instead associated with the dimensionality of the reactor model. Previous one- and two-dimensional MSR comparisons for tube diameters bracketing the 25 mm reference value adopted here provide a benchmarking basis for the use of a cross-sectionally averaged formulation for integral steady-state reactor calculations [36,59], whereas the two-dimensional formulation resolves local radial fields. Radial resolution becomes particularly relevant when local temperature extrema, spatially non-uniform heating, or transient behaviour are of interest [60]. Accordingly, the one-dimensional formulation was adopted for the present comparative steady-state assessment, while higher-dimensional transient modelling is identified as a relevant extension for investigating local gradients during shipboard load transitions.

The resulting governing equations (Equation (1)) are solved in the

form of coupled differential-algebraic equations (DAEs), enabling the prediction of axial temperature profiles, methanol conversion, hydrogen production, and pressure drop under different operating conditions and heating strategies [45]. Additional information on assumptions, models, and coefficients relevant for methanol steam reforming modelling is reported in Section S1 of the Supplementary Material, in agreement with the current literature [48,49,61,62].

$$\left\{ \begin{array}{l} v_z \frac{dC_y}{dz} = \sum_{r=1}^{N_r} \nu_{y,r} \eta_r \rho_{\text{bulk}} S_{\text{BET}} \mathcal{R}_r \quad \forall y \in [1, N_{\text{comp}}] \\ 0 = -k_{m,y} a_{\text{part}} (C_y - C_{y,\text{surf}}) + \sum_{r=1}^{N_r} \nu_{y,r} \eta_r \rho_{\text{bulk}} \mathcal{R}_r (T_{\text{surf}}, C_{i,\text{surf}}) \quad \forall y \in [1, N_{\text{comp}}] \\ v_z \rho \hat{C}_p \frac{dT}{dz} = \sum_{r=1}^{N_r} \eta_r \rho_{\text{bed}} \mathcal{R}_r (-\Delta \tilde{H}_r) - \frac{4U}{D} (T - T_{\text{wall}}) \\ 0 = -h_T a_{\text{part}} (T - T_{\text{surf}}) + \sum_{r=1}^{N_r} (-\Delta \tilde{H}_r) \eta_r \rho_{\text{bed}} \mathcal{R}_r (T_{\text{surf}}, C_{i,\text{surf}}) \\ \frac{dP_{\text{tubes}}}{dz} = -\frac{v_z}{\rho d_{\text{part}}} \left(\frac{1 - \varepsilon_{\text{bed}}}{\varepsilon_{\text{bed}}^3} \right) \left[\frac{150(1 - \varepsilon_{\text{bed}})\mu}{d_{\text{part}}} + 1.75v_z \right] \end{array} \right. \quad (1)$$



The modelling framework underlying the present one-dimensional MSR formulation was previously assessed through a hierarchical validation and benchmarking procedure. First, the parent two-dimensional model, based on the same reaction kinetics, effectiveness-factor treatment, mass and energy balances, and wall-to-bed heat-transfer description, was validated against experimental measurements under both steady-state and dynamic conditions [60]. The model reproduced the measured internal reactor-temperature profiles with maximum local deviations of approximately 15 K. Quantitative steady-state validation of outlet composition was available for CO at seven combinations of reactant throughput and electrical heating power. Based on the data reported in Table 6 of [60], the mean absolute relative deviation between the simulated CO concentration and the midpoint of the corresponding experimental range was approximately 10%, with a maximum deviation of approximately 25%. Three of the seven predictions fell within the measured ranges, whereas the remaining four were below the corresponding lower limits by no more than 0.051 mol m⁻³. The transient validation also reproduced the temporal evolution of H₂, CO₂, and CO concentrations, although component-specific quantitative error metrics were not reported in Ref. [60].

The one-dimensional steady-state formulation was subsequently benchmarked against the two-dimensional model for tube internal diameters of 20 and 30 mm, bracketing the 25 mm reference diameter adopted in the present study [59]. In this benchmark, the thermal boundary conditions of the two formulations were independently adjusted to achieve the same target outlet methanol conversion of 95%. Agreement in conversion was therefore imposed by the benchmark protocol and cannot be interpreted as an independent prediction-error metric. The comparison instead quantified the effect of radial resolution on the reactor thermal requirements. Relative to the one-dimensional formulation, the two-dimensional model required approximately 3.8–13.5% higher flue-gas mass flow rates and predicted flue-gas outlet temperatures 5–18 K higher across the investigated cases. These discrepancies increased from the 20 mm to the 30 mm tubes, consistently with the increasing influence of radial heat-transfer resistance resolved by the two-dimensional formulation. A separate quantitative deviation for steady-state selectivity was not reported in Ref. [59]

and is therefore not claimed here. Overall, the benchmark provides quantitative support for using the one-dimensional formulation for comparative integral steady-state calculations, while showing that local radial temperature fields and the heat-transfer duty required to achieve a prescribed conversion are more accurately resolved by the two-dimensional model.

The experimental validation in Ref. [60] employed electrical wall heating and therefore provides direct experimental evidence for the electrically heated reactor and wall-to-bed heat-transfer formulation. The flue-gas heat-transfer formulation was exercised in the one- and two-dimensional numerical benchmark of [59], but no independent experimental validation of the complete flue-gas-heated configuration is claimed. Condensing-steam heat transfer is described using the classical Nusselt film-condensation correlation within its conventional applicability assumptions; marine-motion-induced film redistribution and transient condensate dynamics are not resolved by the present steady-state formulation.

Pressure drop was calculated using the Ergun correlation for packed beds. Its applicability was checked against the catalyst-particle size, bed voidage, tube-to-particle diameter ratio, and particle Reynolds-number range encountered across the investigated configurations and operating conditions, as summarised in Table S5. These checks support its use as a correlation-based engineering estimate within the investigated conditions. However, no configuration-specific experimental validation of the predicted pressure drops was available, and the pressure-drop results should therefore not be interpreted as independently validated predictions.

A structured summary of the experimental validation, numerical benchmarking, correlation-applicability evidence, and associated limitations for the reactor model, heat-transfer formulations, and pressure-drop calculation is provided in Section S2.5 and Table S5 of the Supplementary Material. This evidence supports the use of the adopted formulations within the investigated conditions but should not be interpreted as a formal uncertainty or parameter-sensitivity analysis of the kinetic and heat-transfer models.

2.3. Thermal management and reactor design

Three alternative heating configurations are investigated in this work: Joule-heated walls, flue-gas heating, and condensing-steam heating. In the Joule-heated configuration (A), heat is generated uniformly within the reactor walls and transferred directly to the catalyst-packed tubes. An additional wall energy balance is therefore introduced to account for the coupling between electrical heat generation and heat transfer to the reacting mixture. The resulting steady-state wall balance is reported in Equation (5) and follows modelling approaches commonly adopted for electrified reactors [63]. FeCrAl tubes are assumed to ensure electrical conductivity and stable resistivity under operating conditions [64].

$$0 = -\frac{4DU}{t_w(2D + t_w)}(T_{\text{wall}} - T) + \frac{16\rho_{e,\text{wall}}I^2}{\pi^2 t_w^2 (2D + t_w)^2} \quad (5)$$

For the flue-gas-heated configuration, thermal energy is supplied by a hot gas stream flowing on the shell side. Heat transfer is described through shell-side energy and momentum balances, accounting for convective heat transfer and pressure losses within the shell-and-tube geometry. This configuration is representative of reforming systems integrated with onboard combustion-based units or waste-heat recovery systems [65–67]. The shell-side energy and momentum balances are reported in Equations (6) and (7), respectively.

$$v_{z,\text{shell}} \rho_{\text{shell}} \hat{C}_{p,\text{shell}} \frac{dT_{\text{shell}}}{dz} = N_t \frac{4U}{d_{\text{ext}}} (T - T_{\text{shell}}) \quad (6)$$

$$\frac{dP_{\text{shell}}}{dz} = -\frac{(2 + N_b)\rho_{\text{shell}}v_{z,\text{shell}}^2}{2L_{\text{tot}}} - \frac{4f(N_b + 1)}{d_{\text{eq}}} d_{\text{shell}} \rho_{\text{shell}} \frac{v_{z,\text{shell}}^2}{4L_{\text{tot}}} \quad (7)$$

In the condensing-steam configuration, heat is supplied through the condensation of saturated steam on the shell side. The shell-side section is therefore modelled analogously to a shell-and-tube condenser operating under film-condensation conditions. Horizontal tubes are assumed to reduce condensate-film thermal resistance and enhance heat-transfer performance, in line with Nusselt condensation theory [68]. Owing to the latent-heat-driven nature of condensation, the shell-side temperature is assumed equal to the local steam saturation temperature and no shell-side energy balance is required. Instead, steam consumption is evaluated through the mass balance reported in Equation (8).

$$\frac{dm_{\text{steam}}}{dz} = -\frac{\pi d_{\text{ext}} N_t U}{\Delta \hat{H}_{\text{vap}}} (T_{\text{shell}}^{\text{eq}} - T) \quad (8)$$

Equation (8) is based on classical Nusselt film-condensation theory for horizontal tubes under quiescent conditions. Under shipboard operation, pitching, rolling, and vibration may alter the effective gravity field and, consequently, the distribution and drainage of the condensate film. Because the liquid film represents the dominant thermal resistance during filmwise condensation, motion-induced waviness, thinning, redistribution, or droplet detachment may locally enhance condensate removal and heat transfer. Conversely, motion opposing drainage may promote local film thickening, pooling, or uneven tube-bundle inundation, thereby reducing the instantaneous heat-transfer coefficient and inducing fluctuations in the transferred heat flux. Vibrational excitation may likewise affect condensate detachment and liquid redistribution, with the resulting response depending on the amplitude, frequency, and direction of the imposed motion, as well as on tube orientation, surface wettability, and bundle geometry. Accordingly, the net effect of marine motion cannot be assumed to be exclusively beneficial or detrimental. The present steady-state model therefore adopts the conventional quiescent Nusselt correlation as a baseline heat-transfer description. Quantification of motion-induced condensation effects would require dedicated transient multiphase simulations and/or experiments under representative marine-motion conditions.

The design procedure involves the variation of key design variables, including reactor length, number of tubes, and heating intensity, depending on the selected heating strategy. Preliminary geometrical constraints relevant to shipboard integration are included in the reactor-design screening, including a maximum allowable reactor height of approximately 2.5 m and limits on the overall equipment dimensions. Tube lengths between 1 m and 6 m are considered, with extensions up to 12 m included as process-design candidates. These geometrical constraints are intended to restrict the investigated design space but do not constitute a mechanical, manufacturing, or installation qualification of the resulting reactor configurations. Additional engineering constraints are imposed to ensure acceptable thermal and fluid-dynamic performance. Reactor aspect ratios are restricted between 2 and 5 to avoid excessive pressure losses or flow maldistribution, while a triangular tube arrangement with a pitch equal to 1.25 times the tube outer diameter is adopted throughout the analysis. A reference tube diameter of 25 mm is used, consistent with the commonly reported 20–30 mm range for tubular MSR reactors [36].

Different shell-side arrangements are considered depending on the selected heating strategy, consistently with standard shell-and-tube engineering practices and TEMA recommendations. Flue-gas-heated configurations are operated in co-current mode to improve thermal matching along the reactor axis [69], whereas condensing-steam systems are limited to single-pass shell arrangements to facilitate condensate drainage. Once a process-design-feasible reactor configuration is identified at the nominal operating condition, the reactor geometry is kept fixed and the system is evaluated under all other operating regimes by varying only the operating variables. No explicit optimization algorithm is employed; instead, the reactor design space is explored through a parametric analysis to identify configurations satisfying the adopted process, thermal, geometrical, and fluid-dynamic constraints.

2.4. Sustainability assessment framework

The performance of the investigated reactor configurations is evaluated through a key performance indicator (KPI)-based sustainability framework aimed at enabling a consistent comparison among alternative heating strategies under variable shipboard operating conditions. All KPIs are defined according to a higher-is-better convention, such that increasing indicator values correspond to improved sustainability performance. Dimensional indicators for four complementary domains are considered: technological performance (Tech), economic viability (Eco), environmental impact (Env), and safety (Safe) [70–72].

2.4.1. Technological indicator

The technological indicator quantifies the capability of each reactor configuration to produce hydrogen while maintaining favourable thermal conditions within the catalytic bed. The indicator combines three contributions: (i) the distance from the catalyst deactivation temperature ΔT_d , (ii) the hydrogen production rate ($\dot{m}_{H_2}$), and (iii) a temperature-profile score (T_{score}).

$$Tech = \Delta T_d \cdot \dot{m}_{H_2} \cdot T_{score} = (T_{min} - T_d) \cdot \dot{m}_{H_2} \cdot T_{score} \quad (9)$$

where T_{min} is the minimum temperature observed along the reactor axis and $T_d = 420$ K is the catalyst deactivation threshold. The temperature-profile score is defined as:

$$T_{score} = \sum T_i \cdot s_i \quad (10)$$

where s_i is a weighting factor associated with the temperature interval in which the local temperature T_i falls, in comparison with the temperature range between the catalyst deactivation temperature T_d and the target operating temperature $T_{opt} = 523$ K ($s_1 = 1$, $s_2 = 1/2$, $s_3 = 1/3$ and $s_4 = 1/4$). An additional overheating interval is assigned a weighting factor equal to zero in order to penalize excessive temperatures. A schematic representation of the adopted scoring procedure is reported in Fig. 2.

2.4.2. Economic indicator

The economic indicator Eco is defined as the inverse of the discounted life-cycle cost (LCC), such that lower life-cycle costs correspond to higher indicator values. The LCC includes capital expenditure (CAPEX) and discounted operating expenditure (OPEX) over the system lifetime [73], according to:

$$Eco^{-1} = LCC = CAPEX + \sum_{t=1}^n \frac{OPEX_t}{(1+r)^t} \quad (11)$$

where n is the system lifetime and r is the discount rate. In the present work, a system lifetime of 25 years and a discount rate of $r = 6\%$ are assumed [74]. Because the discount rate determines the present value of future operating expenditures, variations in r may affect the relative economic performance of configurations characterised by different CAPEX/OPEX distributions. A sensitivity analysis was therefore performed by varying r from 4% to 10%, while keeping the system lifetime, CAPEX and OPEX assumptions, and all technical, environmental, and safety inputs unchanged. For each value of r , the economic indicator, normalized economic KPI, and aggregated sustainability indicators were recalculated for all configurations. The complete results are reported in Section S5 of the Supplementary Material.

CAPEX includes reactor and catalyst costs. Reactor costs are estimated using standard equipment-cost correlations [75], while material-dependent correction factors are introduced to account for the different construction materials associated with each heating strategy, as detailed in Section S2.1 of the Supplementary Material. Operating expenditures include methanol consumption and electricity requirements. Methanol is considered both as reactant and auxiliary fuel, with a reference price of 0.481 \$ kg⁻¹ [76], while electricity consumption accounts for pumps, compressors, and Joule-heating duties, using a reference cost of 0.255 \$ kWh⁻¹ [77]. Water purchase cost is excluded from the operating expenditures because, under the adopted process-balance and recovery assumptions, the internally recovered water is sufficient to satisfy the reforming-water requirement.

2.4.3. Environmental indicator

The environmental indicator Env (Equation (12)) is defined as the inverse of the greenhouse-gas intensity GHG_{int} , such that lower emissions correspond to higher environmental performance. The GHG intensity combines direct process-emission contributions and indirect contributions associated with the mass and energy flows included within the adopted reactor-centred assessment boundary, using the emission factors reported in Table 2. Additional details on the calculation procedure are provided in Section S2.2 of the Supplementary Material.

$$Env^{-1} = GHG_{int} = \dot{m}_{CO_2,eq}^{(1)} + \dot{m}_{CO_2,eq}^{(2)} \quad (12)$$

The methanol and electricity emission factors reported in Table 2 define the reference scenario adopted in the present assessment. The

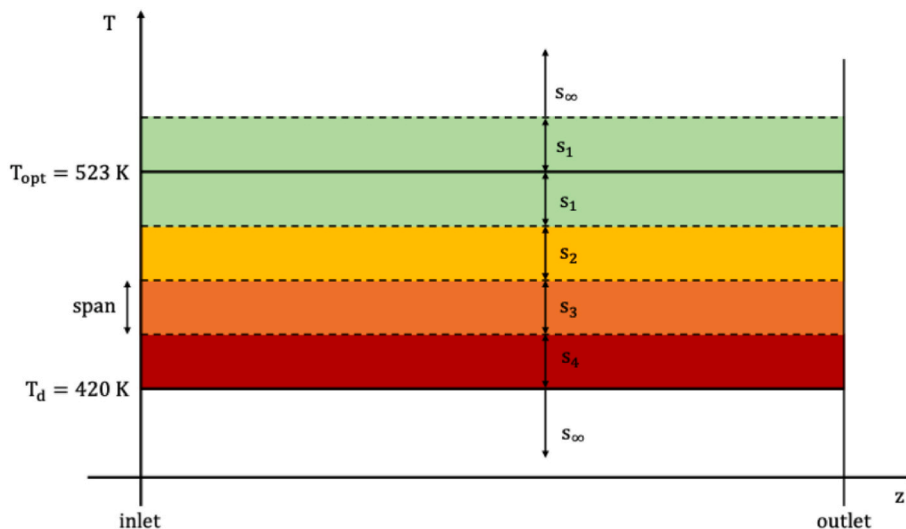


Fig. 2. Schematic representation of the temperature intervals and weighting factors adopted for the calculation of the temperature-profile score T_{score} . Temperatures within the desired operating range receive progressively decreasing weights, whereas overheating conditions are assigned a zero score.

Table 2

Emission factors adopted in the present work [78,79].

Emission source	Methanol	Water	Carbon dioxide	Carbon monoxide	Nitrogen	Electricity
Emission factor	0.7	0.002	1	0	0	0.42
Units	$\frac{\text{kg}_{\text{CO}_2,\text{eq}}}{\text{kg}_{\text{CH}_3\text{OH}}}$	$\frac{\text{kg}_{\text{CO}_2,\text{eq}}}{\text{kg}_{\text{H}_2\text{O}}}$	$\frac{\text{kg}_{\text{CO}_2,\text{eq}}}{\text{kg}_{\text{CO}_2}}$	$\frac{\text{kg}_{\text{CO}_2,\text{eq}}}{\text{kg}_{\text{CO}}}$	$\frac{\text{kg}_{\text{CO}_2,\text{eq}}}{\text{kg}_{\text{N}_2}}$	$\frac{\text{kg}_{\text{CO}_2,\text{eq}}}{\text{kWh}}$

implications of replacing the conventional-methanol factor with pathway-specific values representative of renewable methanol are discussed in Section 3.5. Because the vessel is modelled as an isolated energy system, electricity consumed by the reforming subsystem must be supplied by the onboard energy network and is therefore not treated as an emission-free utility. Within the adopted reactor-centred boundary, the associated GHG burden is accounted for as an indirect contribution by applying an electricity emission factor of $0.42 \text{ kgCO}_2\text{-eq kWh}^{-1}$. This value is used as a reference scenario proxy for the GHG burden associated with supplying electricity to the reforming subsystem; the specific onboard generation technology and its part-load behaviour are not explicitly modelled. The same emission factor is applied to the electricity consumption of all configurations. Its greater influence on the Joule-heated configurations therefore arises from their higher electrical demand rather than from a technology-specific factor. However, the adopted value is scenario-dependent, and the resulting environmental ranking should not be interpreted as universal. A lower-carbon onboard electricity pathway would reduce the indirect GHG contribution associated with Joule heating and could modify the relative environmental differences among the investigated heating strategies.

To quantify the dependence of the results on this assumption, a post-processing sensitivity analysis was performed by varying the electricity emission factor from 0.02 to $0.82 \text{ kgCO}_2\text{-eq kWh}^{-1}$ while retaining the previously calculated reactor outputs and electricity requirements unchanged. For each emission-factor scenario, the electricity-associated GHG contribution, the normalized environmental KPI, and the aggregated sustainability indicators were recalculated under all decision-making perspectives and using both additive and geometrical aggregation. The complete post-processing procedure, rationale for the selected scenario-bounding range, and results are reported in Section S6 of the Supplementary Material.

2.4.4. Safety indicator

The safety domain is represented through an intrinsic safety indicator based on the Dynamic Fire and Explosion Index (DF&EI) [72]. The DF&EI was selected because it enables a consistent comparison among alternative reactor configurations without requiring detailed process-specific information, making it suitable for recursive multi-criteria assessments involving a large number of design alternatives. The safety indicator is defined as:

$$Safe = DF\&EI^{-1} \quad (13)$$

such that lower fire and explosion hazards correspond to higher safety performance. For the Joule-heated configuration, the heat-supply mechanism does not involve an additional shell-side process-fluid inventory or pressurised stream. Consequently, the DF&EI calculation does not include contributions associated with shell-side material inventory, leakage, or pressurised release. The energetic contribution associated with electrical heat generation is nevertheless retained through an additional exothermic-process factor adopted in the DF&EI calculation (Section S2.3). Thus, the safety evaluation of the Joule-heated configuration does not rely solely on the absence of a shell-side material stream.

The DF&EI does not, however, explicitly account for the probability of electrical-equipment failure or for marine-specific electrical degradation and failure mechanisms, including water ingress, saline contamination, insulation degradation, electrical tracking, short circuits, arc faults, and vibration-induced damage. Quantitative assessment

of these hazards would require design-specific information on the electrical architecture, voltage and current levels, power-conversion and protection systems, insulation and enclosure characteristics, equipment location and environmental qualification, together with appropriate component-reliability data. Because these details are not defined at the conceptual design stage considered here, the reported safety indicator should be interpreted as a comparative intrinsic fire-and-explosion hazard metric rather than as a comprehensive probabilistic assessment of marine electrical risk.

2.4.5. Aggregation and normalisation procedures

To account for the variable-load nature of shipboard operation, the dimensional indicators calculated for each operating regime are averaged using weighting factors proportional to the corresponding operating time shares, reported in Section S2.4 of the Supplementary Material, to obtain an aggregated value for each domain. The resulting indicators are subsequently normalized with respect to the best-performing configuration within each assessment domain (i.e., the one represented by the maximum value of the calculated indicator). The resulting normalized KPIs range between 0 and 1, allowing the direct comparison and aggregation of indicators belonging to different sustainability domains.

The normalized KPIs (Equation (14)) are then combined into aggregated sustainability scores to allow the ranking of investigated configurations. Both additive and geometric aggregation procedures were employed. Four alternative weighting policies are considered to represent different decision-making perspectives: individualist, egalitarian, hierarchist, and equal-weighting [37]. The corresponding weighting factors are reported in Section S2.4 of the Supplementary Material.

$$\begin{cases} KPI_{add} = \sum \omega_{KPI,m} \cdot KPI_m \\ KPI_{geo} = \prod KPI_m^{\omega_{KPI,m}} \end{cases} \quad (14)$$

where KPI_m is the normalized indicator associated with the m -th sustainability domain and $\omega_{KPI,m}$ is the corresponding weighting coefficient. A schematic representation of the sustainability assessment is reported in Fig. 3.

It should be emphasised that the normalized KPIs and the resulting aggregated sustainability indicators are comparative measures defined with respect to the best-performing alternatives within the investigated candidate set. Consequently, values approaching unity indicate proximity to the best available configuration under the adopted system boundaries, weighting policy, and aggregation procedure; they should not be interpreted as evidence of an absolute sustainability level or compliance with an external sustainability threshold.

All configurations satisfying the adopted process, thermal, geometrical, and fluid-dynamic constraints, together with the preliminary size-envelope constraints relevant to shipboard integration, were retained in the sustainability assessment. The resulting feasible design set comprised 36 auxiliary-system and 27 propulsion-system configurations. KPI normalisation, weighting, and aggregation were performed using this complete set. For detailed presentation in the main text, configurations were subsequently selected within each heating-strategy and power-application family when they achieved the highest aggregated sustainability indicator under at least one combination of decision-making perspective and aggregation method. This selection was performed exclusively for reporting purposes and did not affect the

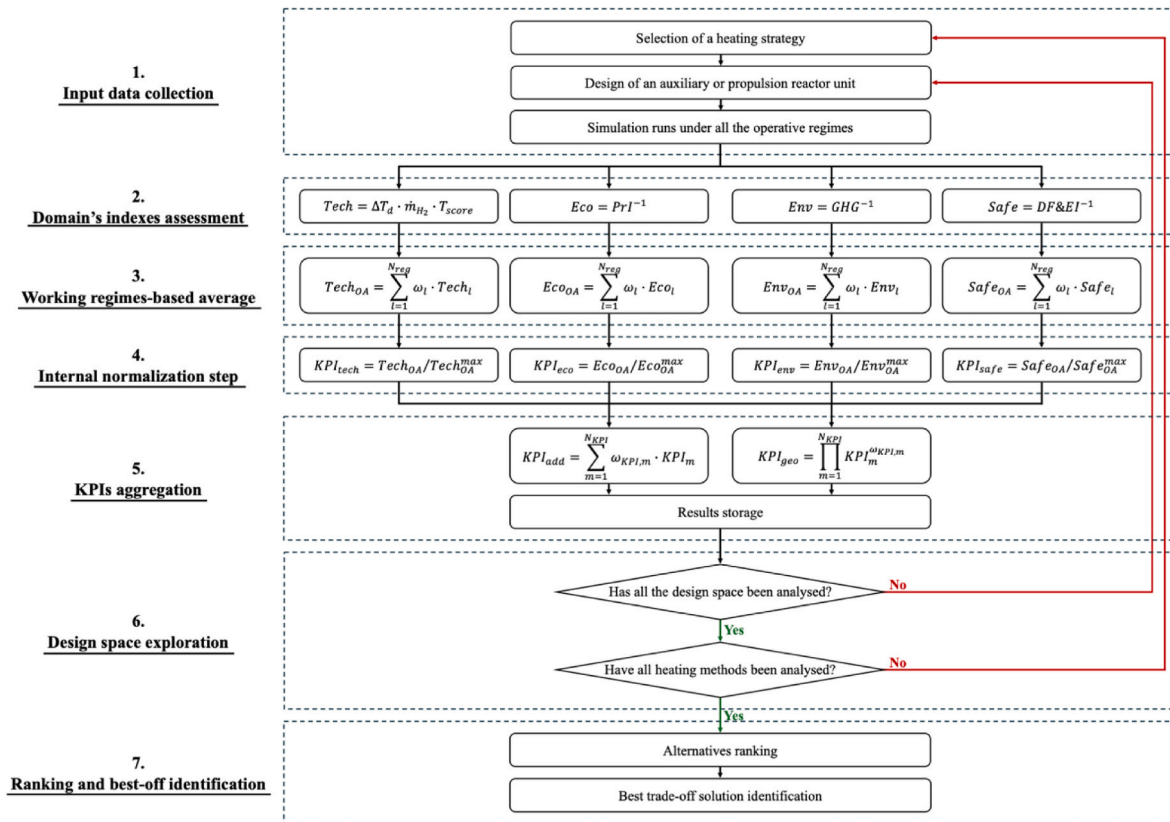


Fig. 3. Schematic representation of the sustainability-assessment framework adopted in this work, including KPI calculation, normalisation, operating-regime aggregation, weighting-policy application, and final KPI aggregation.

underlying KPI calculations, normalisation procedure, or ranking of the complete feasible design set.

3. Results and discussion

Application of the process, thermal, geometrical, and fluid-dynamic constraints, together with the preliminary shipboard size-envelope constraints described in Section 2.3, resulted in 36 process-design-feasible configurations for the auxiliary system and 27 for the propulsion system. Their complete reactor-design characteristics are reported in Section S3, while the corresponding sustainability-assessment results for the full candidate set are provided in Section S4 of the Supplementary Material. To maintain a concise comparison in the main text,

Table 3 reports only the 11 unique configurations that achieved the highest aggregated sustainability score within their respective heating family and application under at least one weighting policy or aggregation procedure. Thus, the configurations omitted from Table 3 were not excluded from the assessment but only from the detailed main-text presentation.

3.1. Sustainability assessment

The aggregated KPIs obtained under the different decision-making policies are reported in Table 3. The configurations presented individually in the main text were selected only after completing the sustainability assessment for the entire feasible design set. For each heating

Table 3

List of the aggregated KPIs obtained in this work applying different decision-making perspectives for the highest-performing solutions within each heating strategy. The best overall reactor configurations are shown in bold.

ID	Individualist		Egalitarian		Hierarchist		Equal weighting	
	$KPI_{add} [-]$	$KPI_{geo} [-]$	$KPI_{add} [-]$	$KPI_{geo} [-]$	$KPI_{add} [-]$	$KPI_{geo} [-]$	$KPI_{add} [-]$	$KPI_{geo} [-]$
Joule-heated reactor								
A3	-	-	0.678	0.640	0.744	0.709	-	-
A4	0.870	0.840	-	-	-	-	-	-
A6	-	-	-	-	-	-	0.700	0.658
P1	-	-	0.699	0.672	0.756	0.731	0.719	0.687
P4	0.875	0.849	-	-	-	-	-	-
Flue-gas-heated reactor								
A11	0.962	0.962	-	-	0.922	0.922	0.934	0.934
A12	-	-	0.915	0.915	-	-	-	-
P10	0.953	0.951	0.870	0.867	0.894	0.891	0.900	0.896
Condensing-steam-heated reactor								
A36	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
P25	0.998	0.998	-	-	0.998	0.998	0.997	0.997
P27	-	-	0.998	0.998	-	-	-	-

strategy and power application, a configuration was retained if it achieved the highest aggregated sustainability score under at least one of the four weighting policies using either the additive or geometrical aggregation procedure. Selection was performed using the unrounded indicator values, while duplicate configurations selected under multiple perspectives were counted only once. This best-in-family procedure resulted in 11 representative configurations: A3, A4, A6, A11, A12, and A36 for the auxiliary system, and P1, P4, P10, P25, and P27 for the propulsion system. No Pareto-optimality screening or additional subjective engineering selection was applied at this stage. The complete KPI results for all feasible configurations are reported in Section S4 of the Supplementary Material.

In all cases, additive and geometric methods identify the same best-performing configurations, while numerical differences between the corresponding aggregated indicators remain limited and progressively decrease for higher sustainability levels. The results also indicate a consistent trend across all decision-making perspectives. Although the absolute KPI values vary depending on the relative importance assigned to technological, economic, environmental, and safety criteria, the same overall ranking of heating strategies is systematically obtained. Indeed, condensing-steam-heated reactors achieve the highest aggregated sustainability indicators for both auxiliary and propulsion applications, whereas flue-gas-heated configurations exhibit intermediate performance, and Joule-heated reactors display the lowest sustainability scores. The preservation of this ordering across the investigated weighting perspectives and aggregation procedures indicates that, within the adopted candidate set and decision rules, the technology ranking is not strongly affected by the stakeholder-weighting choices considered in this work. The influence of the weighting policy becomes more appreciable when comparing configurations within the same heating family (Section S4 of the Supplementary Material). This effect is most evident for the Joule-heated reactors, for which different stakeholder perspectives lead to the selection of different highest-ranking configurations, indicating more pronounced trade-offs among sustainability domains. In contrast, the condensing-steam-heated reactors show almost complete agreement among the investigated weighting policies, with configuration A36 consistently selected for auxiliary applications and only negligible differences between propulsion configurations P25 and P27.

The sensitivity of the ranking to the economic assumptions was further examined by varying the discount rate over the range $r = 4\text{--}10\%$. Across this interval, both the economic ordering of the three heating

strategies and the overall sustainability ranking remained unchanged. Although the normalized economic KPI varied because of differences in the CAPEX/OPEX distributions of the configurations, condensing-steam heating retained the highest ranking, followed by flue-gas and Joule heating, for both auxiliary and propulsion applications. These results indicate that the technology ordering is insensitive to the discount rate within the investigated range. Complete results are reported in Section S5 of the Supplementary Material.

Additional insight into the sustainability ranking can be obtained from the radar plots reported in Fig. 4, which compare the normalized domain-specific KPIs of the highest-performing configuration associated with each heating strategy. For both auxiliary and propulsion applications, Fig. 4 reveals three distinct sustainability profiles. Joule-heated reactors exhibit the lowest technological and economic indicators, while maintaining comparatively high environmental and safety performance. This behaviour suggests that the main limitations of electrified solutions originate from thermal-management and economic aspects rather than from environmental or safety considerations.

Flue-gas-heated reactors display a more balanced sustainability profile, with technological, economic, and environmental KPIs generally clustered between 0.85 and 0.95. The only noticeable reduction is observed for the safety indicator, reflecting the presence of high-temperature combustion products and the associated operational hazards. Condensing-steam-heated reactors achieve consistently high values across all sustainability domains, generating the most uniform profiles among the investigated technologies. This behaviour is observed for both auxiliary and propulsion applications and is consistent with the limited sensitivity of their relative ranking to the weighting policies investigated in this work. In particular, the nearly overlapping profiles of configurations P25 and P27 further confirm the limited influence of stakeholder preferences on the final assessment.

Fig. 5 provides information on the distribution of the sustainability indicators across the complete set of feasible reactor designs considered in the assessment. The technological and economic KPIs exhibit the largest variability across the investigated configurations, whereas the environmental and safety indicators remain comparatively concentrated at higher values. A comparison among the heating strategies also reveals differences in the sensitivity of the predicted performance to the geometrical and operating variables explored in the design space. Joule-heated reactors exhibit comparatively narrow KPI distributions, although at generally lower technological and economic performance levels. Flue-gas-heated reactors achieve higher and more balanced

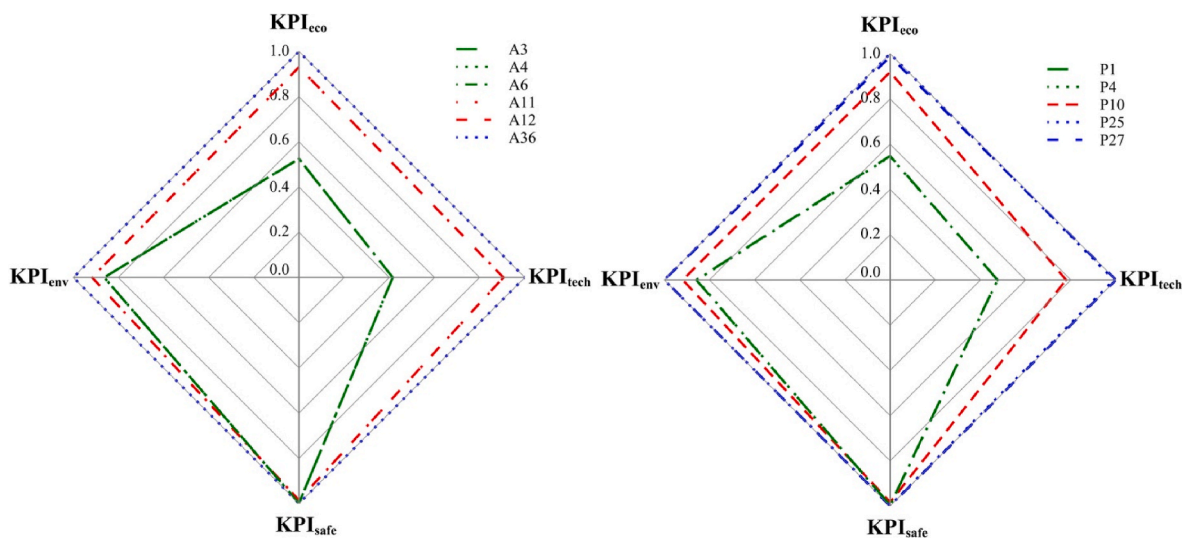


Fig. 4. Comparison of the normalized sustainability-domain KPIs for the highest-performing reactor configurations associated with each heating strategy. Results are reported for auxiliary (left) and propulsion (right) applications. Joule-heated, flue-gas-heated, and condensing-steam-heated reactors are shown in green, red, and blue, respectively. The radar plots provide a visual comparison of the balance among the different sustainability domains.

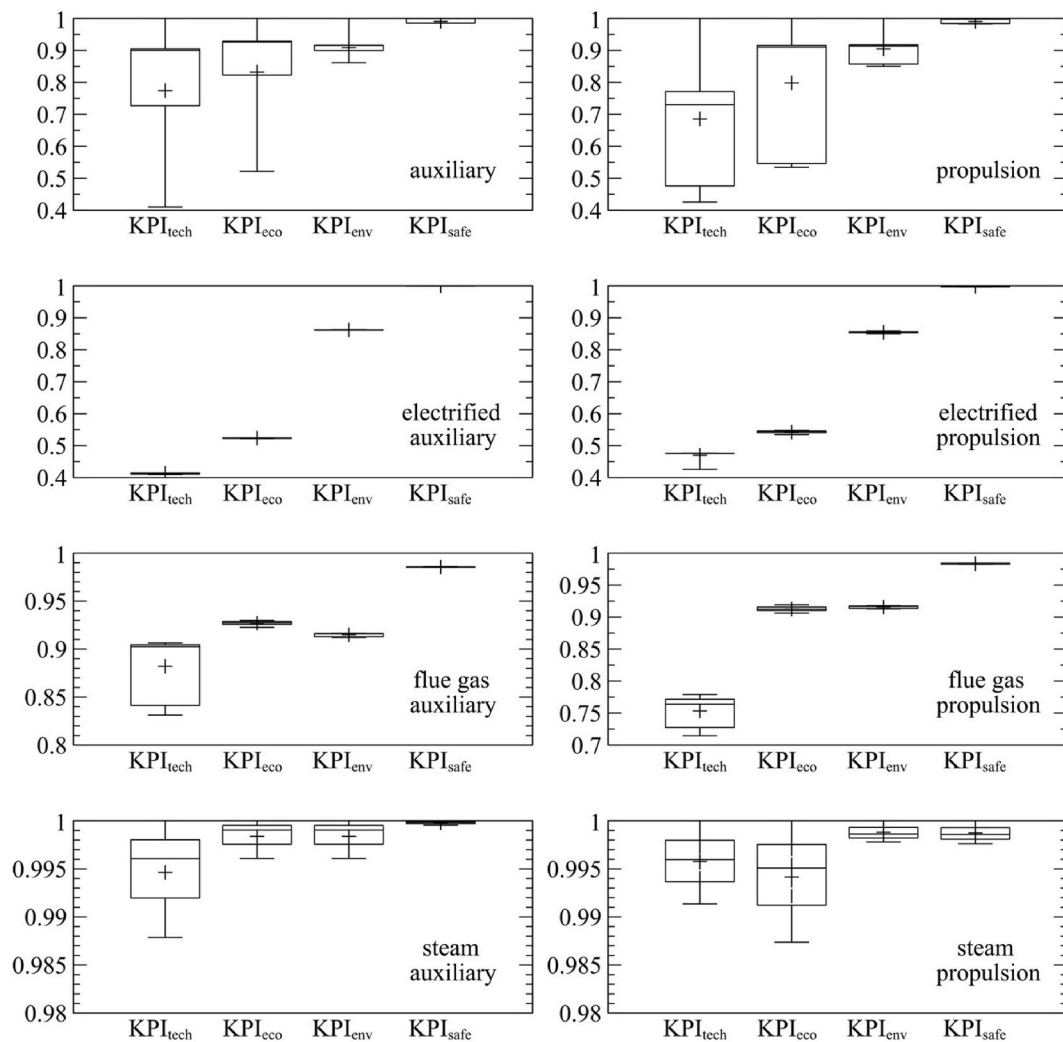


Fig. 5. Boxplot distributions of the normalized technological, economic, environmental, and safety KPIs obtained for all feasible reactor configurations. Results are reported for auxiliary (left column) and propulsion (right column) applications. The first row (Global) refers to the complete dataset irrespective of the adopted heating strategy, whereas the remaining rows report the distributions associated with the Joule-heated, flue-gas-heated, and condensing-steam-heated reactor families. Boxes represent the interquartile range, the central line indicates the median value, and the cross denotes the arithmetic mean. Whiskers correspond to the minimum and maximum values observed within each dataset.

sustainability indicators, while their technological KPI shows a wider dispersion, indicating greater sensitivity to the selected design and operating conditions. The condensing-steam-heated configurations exhibit the smallest variability across the investigated design space, with all sustainability indicators concentrated within a narrow region close to the candidate-set maximum. This result indicates that their favourable relative performance is not limited to a small subset of designs but is maintained across the geometrical alternatives and discrete steady-state conditions explored in the present analysis.

Overall, within the investigated candidate set and under the adopted normalisation procedure, the environmental and safety KPIs show comparatively limited dispersion, whereas the technological KPI spans a substantially wider range, from values below 0.5 for some Joule-heated reactors to values approaching the candidate-set maximum of unity for condensing-steam-heated configurations. This wider spread indicates that differences in technological performance contribute substantially to the relative sustainability ranking and highlights the influence of the heat-supply strategy on the predicted reactor behaviour. Conversely, the narrower KPI distributions observed for some heating families indicate only limited variability across the sampled steady-state design space and should not be interpreted as evidence of broader engineering robustness. The thermal behaviour associated with the three heating strategies is

therefore examined in greater detail in the following section.

3.2. Thermal behaviour of alternative heating strategies

The axial temperature profiles obtained in this work are reported in Fig. 6 for the auxiliary and propulsion systems. To enable a direct comparison among reactors characterized by different dimensions and geometries, the reactor length is expressed in normalized form. A strong similarity among the temperature profiles associated with configurations belonging to the same heating family can be observed, indicating that the steady-state thermal behaviour is primarily governed by the heat-transfer mechanism rather than by the specific reactor design. More importantly, the three heating strategies generate markedly different temperature profiles, resulting in substantially different levels of cold-spot formation, overheating tendency, temperature uniformity, and spatial matching between heat supply and reaction demand. These characteristics directly affect catalyst utilisation and reactor performance.

The most distinctive thermal behaviour is observed for the Joule-heated reactors. Both auxiliary and propulsion configurations exhibit the characteristic U-shaped temperature profile commonly associated with uniformly electrified tubular reactors. Starting from the reactor

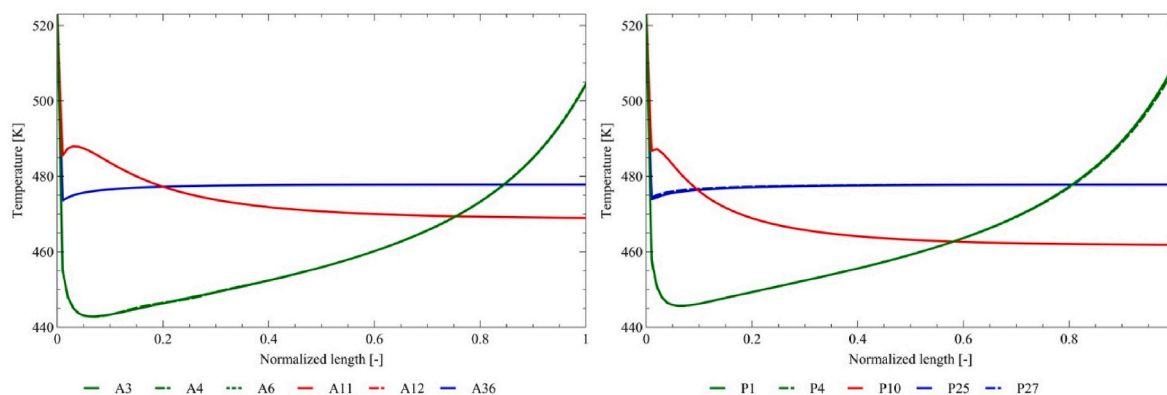


Fig. 6. Axial temperature profiles for the highest-performing auxiliary-system (left) and propulsion-system (right) configurations. Joule-heated, flue-gas-heated, and condensing-steam-heated reactors are shown in green, red, and blue, respectively.

inlet temperature of approximately 523 K, the reacting mixture undergoes a rapid temperature decrease immediately after entering the catalytic section, reaching a minimum temperature of approximately 442–445 K within the first 3–5% of the normalized reactor length.

This pronounced cold spot originates from the strong mismatch between local heat demand and heat supply. At the reactor inlet, methanol and steam concentrations are at their maximum values, resulting in the highest reforming rates and therefore the largest endothermic heat demand along the entire reactor. However, Joule heating generates thermal energy approximately uniformly throughout the reactor wall and is therefore unable to adapt to the strongly non-uniform heat demand associated with the reaction. Consequently, heat is consumed faster than it can be supplied, producing the observed temperature minimum. As methanol conversion increases along the reactor length, the reaction rate progressively decreases, and the local heat demand is reduced. Since electrical heat generation remains essentially constant, the supplied heat flux gradually exceeds the thermal requirements of the reacting mixture, causing the temperature to recover and subsequently increase toward the reactor outlet. The resulting profile highlights a limitation of uniform wall heat generation under the investigated operating conditions: heat supply is comparatively insufficient in the inlet region, where the local endothermic demand is highest, and progressively exceeds the local reaction demand further downstream. This behaviour generates two opposing thermal penalties. On one hand, the severe inlet cold spot reduces catalyst utilisation and increases the deviation from the preferred reforming temperature range. On the other hand, excessive heat supply in the downstream section promotes outlet overheating and deteriorates temperature uniformity along the reactor length. Furthermore, mitigating the latter effect requires reducing the overall electrical heat input, which inevitably intensifies the cold-spot problem. Consequently, a compromise must be established between inlet heat-transfer limitations and outlet temperature control.

Notably, the minimum temperature predicted for the Joule-heated configurations, approximately 442–445 K, remains 22–25 K above the 420 K catalyst-stability criterion adopted in the present assessment and is confined to the first 3–5% of the normalized reactor length. Thus, although the inlet cold spot reduces the local reaction rate and catalyst utilisation, the predicted temperature remains above the stability criterion used in the present evaluation. Moreover, its effect is not assessed solely through the overall methanol conversion: the technological indicator explicitly accounts for both the distance between the minimum reactor temperature and the adopted stability criterion and the deviation of the complete axial temperature profile from the preferred operating range. At the kinetic level, the mechanistically derived Peppley model includes temperature-dependent kinetic, adsorption, and equilibrium terms for methanol steam reforming, methanol decomposition, and the water–gas shift reaction. Consequently, both direct CO formation through methanol decomposition and CO interconversion through

the water–gas shift reaction are represented in the steady-state calculations. A lower local temperature therefore cannot be assumed a priori to increase CO formation, since the resulting CO concentration depends on the relative rates of the competing reaction pathways. Consistently, Agrell et al. [80] reported a strong dependence of CO formation on reactor temperature over Cu/ZnO/Al₂O₃ catalysts and showed that limiting the maximum temperature can suppress CO formation under specific operating conditions, including through reduced contributions from methanol decomposition and reverse water–gas shift. Nevertheless, transient changes in surface coverage, CO-concentration fluctuations, irreversible catalyst deactivation, and catalyst lifetime cannot be quantified using the present steady-state formulation.

A fundamentally different behaviour is observed for the flue-gas-heated reactors. Unlike the electrified systems, these reactors do not exhibit a pronounced U-shaped temperature profile. Instead, the reacting mixture experiences a moderate temperature increase near the reactor inlet, reaching approximately 487–489 K, followed by a gradual decrease toward outlet temperatures between 462 and 470 K. This behaviour originates from the convective heat transfer provided by the shell-side flue-gas stream. At the reactor inlet, the temperature difference between the hot flue gas and the reacting mixture is at its maximum, generating elevated local heat-transfer rates and thereby substantially mitigating the inlet cold spot compared with the Joule-heated configurations. As the flue gas transfers heat to the reactor tubes, its temperature progressively decreases. Simultaneously, methanol conversion increases and reaction rates gradually decline. The combined effect of these phenomena produces the smooth temperature evolution observed along the reactor length. From a thermal-management perspective, this behaviour represents a significant improvement over direct electrical heating. The shell-side fluid naturally delivers larger heat fluxes where the reaction demand is highest and progressively lower heat fluxes downstream, resulting in a better match between heat supply and heat demand. Consequently, both cold-spot formation and outlet overheating are substantially mitigated. Nevertheless, under the investigated configuration, the finite sensible-heat capacity of the flue-gas stream causes the shell-side temperature and the local temperature driving force to progressively decrease along the reactor. As heat is continuously extracted from the shell side, the temperature driving force progressively decreases, reducing the reactor's ability to maintain favourable thermal conditions. Therefore, reactor performance becomes strongly dependent on shell-side operating conditions, including flue-gas flow rate, inlet temperature, and overall heat-transfer coefficient.

The most uniform thermal behaviour is observed for the condensing-steam-heated reactors. Following a limited temperature decrease near the reactor inlet, the reacting mixture approaches an almost constant temperature of approximately 477–478 K, which is maintained throughout most of the reactor length. As a result, the profiles exhibit a

markedly more uniform behaviour than those observed for both Joule-heated and flue-gas-heated configurations. This behaviour is a direct consequence of the latent-heat-driven nature of steam condensation. Unlike sensible heat-transfer media, whose temperature continuously changes as heat is exchanged, saturated steam releases large amounts of thermal energy while remaining essentially at constant temperature. Consequently, the shell side provides an almost isothermal thermal boundary condition along the reactor length. The implications for reactor performance are significant. First, the inlet cold spot is substantially mitigated compared with the Joule-heated reactors, with minimum temperatures remaining approximately 30 K higher than those observed under direct electrical heating. Second, outlet overheating is markedly reduced, since the shell-side temperature remains constrained by the steam-condensation process. As a result, the reacting mixture operates within a much narrower temperature range, improving catalyst utilisation and reducing thermal stresses throughout the reactor. An additional advantage concerns the distribution of the heat flux. At the reactor inlet, where methanol concentrations and reaction rates are highest, the temperature difference between the condensing steam and the reacting mixture is also at its maximum, generating elevated heat-transfer rates. As the reaction progresses and the fluid temperature approaches the steam temperature, the driving force naturally decreases and the local heat flux is reduced accordingly. Therefore, under the simulated steady-state conditions, the condensation mechanism provides a spatially self-matching heat-flux distribution, with the transferred heat decreasing along the reactor as the local temperature driving force and reaction demand decrease. This spatial behaviour should not be interpreted as evidence of dynamic self-regulation.

The observed thermal behaviour is consistent with the high candidate-set-relative technological KPIs and the narrow KPI distributions reported in Fig. 5. In contrast to the other heating technologies, virtually all feasible steam-heated configurations exhibit similar thermal characteristics and achieve very high performance levels. This observation indicates that the favourable sustainability ranking of condensing-steam-heated reactors is not associated with a limited number of optimized designs, but rather reflects the limited sensitivity of the predicted steady-state performance to the geometrical design variables explored in this work.

3.3. Reactor design and operational performance

Table 4 summarizes the principal geometrical and operational characteristics of the highest-performing reactor configurations identified through the sustainability assessment.

Table 4

Main geometrical and operational parameters of the highest-performing reactor configurations, including tube length (L), shell diameter (d_{shell}), tube count (N_t), methanol conversion (χ), and tube-side pressure drop (ΔP). Conversion and pressure-drop values are reported as weighted averages over the complete ship operating profile defined in Table 1.

ID	L [m]	d_{shell} [m]	N_t [–]	χ [%]	ΔP [bar]
Joule-heated reactor					
A3	3.0 (1 pass)	1.22	640	99.3	0.012
A4	4.0 (1 pass)	1.07	480	99.3	0.023
A6	5.0 (1 pass)	0.98	385	99.3	0.038
P1	4.0 (1 pass)	1.98	1820	99.2	0.033
P4	8.0 (1 pass)	1.44	915	99.2	0.170
Flue-gas-heated reactor					
A11	3.0 (2 passes)	1.50	500	99.2	0.019
A12	3.0 (1 pass)	1.09	500	99.1	0.019
P10	6.0 (1 pass)	1.97	1800	99.1	0.057
Condensing-steam-heated reactor					
A36	6.0 (1 pass)	0.86	300	99.5	0.074
P25	6.0 (1 pass)	1.54	1050	99.3	0.119
P27	10.0 (1 pass)	1.22	640	99.3	0.424

For both auxiliary and propulsion applications, weighted methanol conversion remains consistently above 99%, ranging from 99.11% to 99.50%. These limited differences confirm that all heating strategies are capable of satisfying the hydrogen demand imposed by the PEMFC systems. Consequently, the sustainability ranking cannot be attributed to differences in hydrogen productivity or conversion efficiency, but rather to the reactor architectures and engineering solutions required to achieve these performances.

The electrified reactors are characterized by relatively short reactor lengths combined with large tube bundles and shell diameters. Since heat is generated directly within the reactor walls, reactor geometry is not constrained by shell-side hydrodynamics, allowing greater flexibility in the selection of aspect ratio and tube arrangement. This freedom enables compact reactor layouts to be achieved, particularly for auxiliary applications. However, increasing hydrogen demand requires a substantial increase in tube count and shell diameter, as illustrated by the propulsion configurations.

Flue-gas-heated reactors follow a different design philosophy because reactor geometry must simultaneously satisfy tube-side reaction requirements and shell-side fluid-dynamic constraints. In addition to methanol conversion, the shell side must ensure adequate gas distribution, acceptable pressure losses, and sufficient heat-transfer coefficients. As a result, reactor dimensions become strongly coupled to shell-side operating conditions, reducing the geometric flexibility available during the design stage. This behaviour is reflected by the larger shell diameters required to accommodate the flowing heating medium while maintaining acceptable thermal performance.

The condensing-steam-heated reactors exhibit the most distinctive geometric characteristics. For both auxiliary and propulsion applications, the preferred configurations achieve the highest methanol conversions while employing the smallest shell diameters among the investigated technologies. This is achieved by shifting part of the required heat-transfer surface from radial expansion to axial development, resulting in longer reactors with more compact cross-sectional footprints. From a ship-integration perspective, this characteristic is particularly attractive because available installation height is often more restrictive than equipment length. Consequently, horizontal shell-and-tube arrangements can be adopted while maintaining favourable installation dimensions.

The data reported in Table 4 also highlight a clear trade-off between installation footprint and hydraulic performance. Reductions in shell diameter are generally obtained through increases in reactor length, which inevitably increase the pressure drops. This behaviour is particularly evident for the condensing-steam configurations, where extending the reactor length from 6 m (P25) to 10 m (P27) reduces the shell diameter by approximately 20% while increasing the weighted pressure drop from 0.119 bar to 0.424 bar. A similar trend is observed for the electrified reactors. From a hydraulic perspective, even the highest predicted pressure drop remains within the process-design constraints adopted in the present study and therefore does not constitute a limiting hydraulic constraint. However, this hydraulic compatibility does not establish the mechanical or installation feasibility of the reactor. In particular, the 10 m tube length of configuration P27 would require dedicated structural, vibrational, fatigue, and support-design assessment before shipboard implementation.

Another important observation concerns the flexibility of the condensing-steam concept. Configurations P25 and P27 achieve virtually identical methanol conversions despite substantially different reactor geometries. This behaviour indicates that different combinations of reactor length and shell diameter can be adopted without significantly affecting process performance, providing additional freedom during equipment layout and ship integration. Such flexibility is considerably less evident for the flue-gas-heated configurations, whose geometry remains strongly influenced by shell-side flow requirements.

From a mechanical perspective, the 10 m tube length reported for P27 should not be interpreted as a single unsupported structural span. In

a detailed shell-and-tube design, the effective unsupported tube length could be reduced through appropriately spaced support plates, baffles, and, where required, anti-vibration restraints, while the shell and skid structure would require adequate support and stiffening. The detailed design would also need to accommodate differential thermal expansion and ship-induced static and dynamic loads. However, the suitability of any specific support, expansion-compensation, or vibration-mitigation arrangement has not been assessed in the present study. Establishing the mechanical feasibility of P27 would therefore require dedicated structural, modal, and fatigue analyses, including finite-element assessment and verification against the applicable marine classification requirements.

Overall, the reactor-design analysis shows that the investigated heating strategies can achieve comparable methanol-conversion levels through markedly different engineering solutions. The main differences therefore arise from the thermal behaviour, reactor geometry, pressure-drop characteristics, installation requirements, and design flexibility associated with each heat-supply strategy. Within the investigated steady-state design space, condensing-steam heating combines relatively compact reactor dimensions with favourable temperature profiles,

hydraulic performance, and flexibility across the considered operating conditions, providing an engineering basis for its higher aggregate sustainability ranking. The mechanical feasibility of the longest configuration, P27, nevertheless requires dedicated structural and ship-integration assessment. Importantly, the technology-level comparison does not depend uniquely on this configuration. P25 provides a less slender condensing-steam-heated alternative, with a tube length of 6 m and a predicted pressure drop of 0.119 bar, while exhibiting comparable conversion and sustainability performance within the investigated conditions. Therefore, even if P27 were excluded following detailed mechanical qualification, the comparative conclusions regarding condensing-steam heating within the present candidate set would remain unchanged.

3.4. System-level energy integration

Particular attention is devoted to utility requirements, energy recovery, fuel consumption, electrical balances, and greenhouse-gas (GHG) emissions, with the aim of assessing how the selected heating concept influences the integration of the reforming unit within the ship

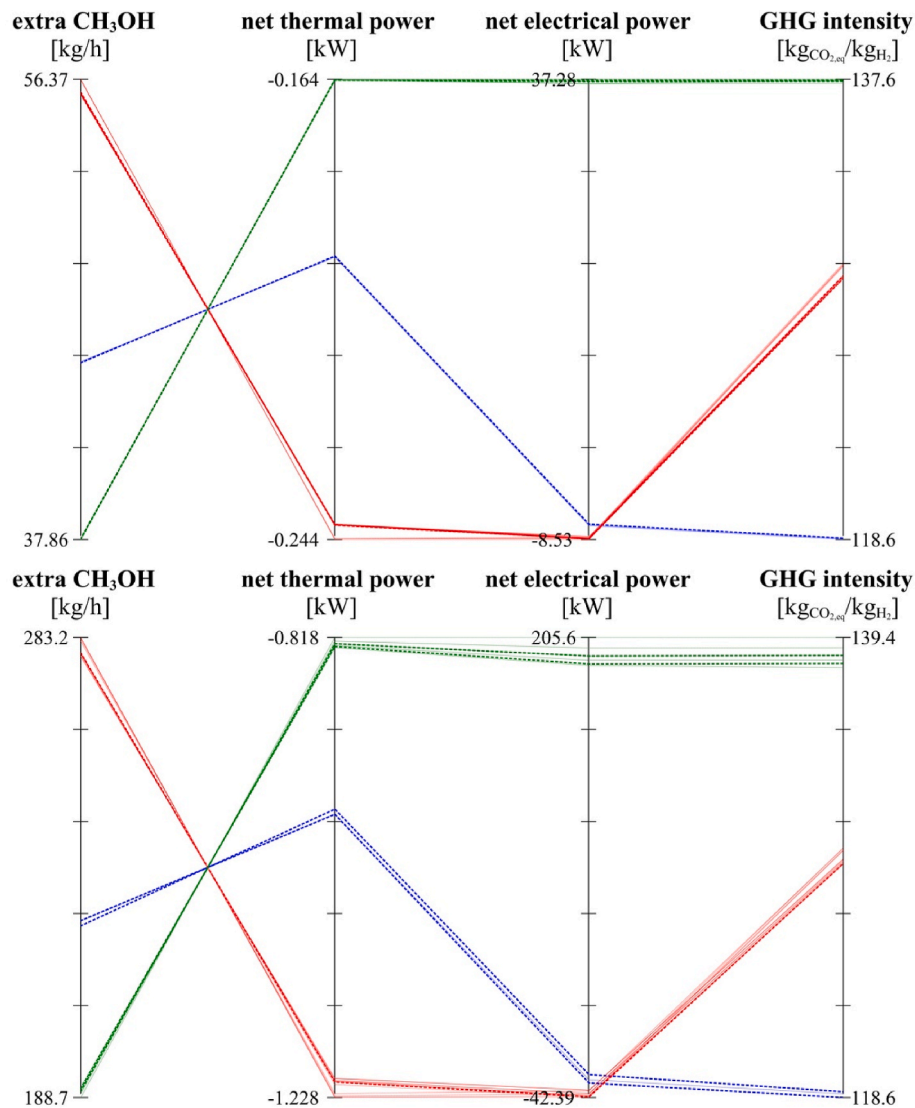


Fig. 7. Parallel-coordinate representation of the principal system-level energy-integration indicators for the best-performing auxiliary (left) and propulsion (right) reactor configurations. The reported variables include additional methanol consumption for utility generation, net thermal duty, net electrical-power balance, and GHG-emission intensity. Joule-heated, flue-gas-heated, and condensing-steam-heated reactors are shown in green, red, and blue, respectively. Within each reactor family, the bold line denotes the highest-performing configuration.

energy system.

To facilitate the comparison, Fig. 7 reports parallel-coordinate plots for the best-performing auxiliary (left) and propulsion (right) configurations. The considered indicators include additional methanol consumption, net thermal-power requirements, net electrical-power balance, and GHG-emission intensity. All values correspond to weighted-average quantities calculated over the complete ship operating profile described in Table 1.

At first sight, the electrified configurations appear favourable because they require the lowest supplementary methanol consumption within the reforming subsystem. This apparent advantage, however, reflects a different allocation of utility demand rather than a lower overall reforming-system energy requirement, since all configurations process similar reactant-methanol quantities and achieve comparable conversion levels. In the Joule-heated configurations, a substantial fraction of the reactor heat duty is supplied as electrical power rather than through thermal utilities. Within the adopted reactor-centred assessment, this electricity consumption is assigned the reference electricity cost and GHG emission factor described in Section 2.4. Consequently, the higher electrical demand of Joule heating contributes to both the economic and environmental indicators. This treatment should not be interpreted as an explicit simulation of a specific onboard generator or of the corresponding ship-level fuel-consumption response.

A markedly different behaviour is observed for the flue-gas-heated and condensing-steam-heated configurations. In these systems, thermal energy can be recovered and redistributed through the heat-integration network incorporated into the process layout. Thermal energy recovered from the catalytic burner, fuel-cell section, and auxiliary units can be reused to satisfy part of the preheating, vaporization, and superheating duties associated with the reforming process, thereby reducing the calculated residual utility requirements.

The influence of heat integration is also reflected in the calculated net electrical-power balance. Whereas the Joule-heated configurations exhibit a net electrical demand, the adopted system-level balances predict a positive net electrical balance for several flue-gas- and condensing-steam-heated configurations as a result of the energy-recovery assumptions and turbine-expander electricity generation included in the model. This quantity represents a potential electrical surplus within the adopted system boundary; its actual export to, or utilisation by, the ship electrical network would depend on the vessel-specific electrical architecture and is not explicitly modelled here. The resulting difference in net electrical demand contributes to the higher calculated economic and environmental indicators of the flue-gas- and steam-heated configurations under the adopted reference assumptions.

Among the investigated alternatives, the condensing-steam-heated configurations exhibit favourable integration characteristics within the adopted energy-balance framework. Condensing steam provides an effective reactor-side heat-transfer mechanism while allowing the thermal duty to be represented through a latent-heat utility interface. Within the assumed heat-recovery architecture, this configuration is associated with comparatively low electrical demand and effective utilisation of the available thermal-energy streams. The detailed generation, conditioning, distribution, and return of the steam utility, however, remain vessel-specific and are outside the present modelling boundary.

These differences are also reflected in the calculated GHG-emission intensities. Under the reference methanol and electricity emission factors adopted in the present assessment, the condensing-steam-heated configurations exhibit the lowest GHG intensities among the investigated alternatives. This result arises from the combined effect of configuration-specific methanol requirements, electrical demand, and the heat-recovery assumptions included within the adopted reactor-centred system boundary. In particular, the comparatively low electrical demand of the steam-heated configurations reduces the electricity-associated indirect GHG contribution under the reference electricity scenario. The resulting environmental differences should therefore be interpreted within the adopted energy-balance assumptions and

emission factors rather than as a direct prediction of total ship-level fuel consumption or emissions.

The same trends are observed for both auxiliary and propulsion applications, although the differences become progressively more pronounced at larger scales. As hydrogen demand increases, utility consumption, heat-recovery opportunities, and electrical-generation potentials scale accordingly, amplifying the benefits associated with effective thermal integration.

Overall, the system-level calculations show that the lower supplementary methanol requirement of the Joule-heated configurations does not translate into the highest economic or environmental indicators within the adopted assessment framework. When the calculated electrical demand, heat-recovery contributions, utility balances, and reference economic and emission factors are considered together, the flue-gas- and particularly the condensing-steam-heated configurations attain higher economic and environmental KPIs. These results remain conditional on the adopted reactor-centred system boundary, heat-recovery architecture, component assumptions, electricity cost and emission factor, and prescribed utility interfaces.

3.5. Discussion

Within the investigated steady-state design space, condensing-steam heating attained the highest aggregate sustainability ranking among the three heating strategies. Beyond the aggregated indicators, the comparison provides several engineering insights relevant to the design and further assessment of shipboard hydrogen-production systems.

3.5.1. Dynamic operation and control implications

A first aspect concerns the potential implications of the heating strategy for future control and load-following operation. Shipboard power demand varies with navigation conditions, hotel loads, manoeuvring operations, and propulsion requirements. However, the present simulations compare independent steady-state operating points and therefore do not quantify response times, control stability, or reactor behaviour during load transitions.

In Joule-heated reactors, electrical power provides a directly adjustable heat input. Previous experimental and numerical studies of ohmically heated reformers have reported high heating rates and close coupling between applied power, reactor temperature, and conversion, suggesting the potential for rapid thermal actuation [81]. Nevertheless, the actual dynamic response depends on reactor geometry, thermal mass, power distribution, and control architecture and cannot be inferred directly for the configurations investigated here. Flue-gas-heated systems would instead be dynamically coupled to the combustion unit supplying the heating medium, requiring coordinated regulation of flue-gas temperature and flow rate; this transient interaction was not evaluated in the present work.

For condensing-steam heating, steam pressure determines the saturation temperature, while steam supply and pressure regulation represent potential manipulated variables for controlling the available thermal duty. These characteristics define possible control degrees of freedom but do not demonstrate rapid response, self-regulation, or stable load-following behaviour. The nearly isothermal temperature profiles and limited performance variability observed here apply only to the investigated discrete steady-state operating points. Establishing the actual controllability of this configuration would require transient modelling of reactor thermal capacitance, steam-system inventories, pressure and flow regulation, condensation behaviour, and condensate drainage.

3.5.2. Model and scenario dependence

The reported rankings also remain conditional on several modelling and scenario assumptions. A formal sensitivity or uncertainty analysis of membrane recovery, kinetic parameters, heat-transfer correlations, and utility-price assumptions was not performed. The kinetic and heat-

transfer formulations are supported by the validation, benchmarking, and applicability evidence described in Section 2.2 and Section S2.5, but this evidence should not be interpreted as a formal parameter-uncertainty analysis. Similarly, the fixed membrane hydrogen-recovery factor of 80% defines a common design assumption, and its influence on the coupled reactor–system design was not quantified. By contrast, the dependence on the discount rate, electricity emission factor, weighting perspectives, and aggregation procedures was explicitly investigated. The resulting rankings should therefore be interpreted within the corresponding model, economic, environmental, and system-boundary assumptions.

3.5.3. Renewable-methanol and electricity scenarios

Transitioning to renewable methanol could substantially reduce the absolute GHG-emission intensities of all investigated configurations, although bio-methanol and e-methanol should not automatically be assigned a zero emission factor. The physical formation and release of CO₂ associated with methanol reforming and auxiliary-fuel conversion remain essentially unchanged on a mass basis, whereas their net climate contribution depends on the origin of the carbon and hydrogen, the energy used for methanol synthesis, and the adopted life-cycle accounting methodology. Pathway-specific Well-to-Tank, Tank-to-Wake, and Well-to-Wake emission factors should therefore be applied consistently with life-cycle GHG assessment approaches for marine fuels [82].

Because the three heating strategies process similar quantities of reactant methanol and achieve comparable conversion levels, reducing the emission factor associated with this common contribution would lower the absolute GHG intensity of all configurations. The remaining relative differences would increasingly depend on configuration-specific auxiliary-methanol and electricity requirements. If methanol were substantially decarbonised while the electricity emission factor remained at its reference value, the electrical demand of Joule heating would account for a larger fraction of the remaining configuration-dependent GHG burden. Conversely, lower-carbon onboard electricity would reduce this contribution and narrow the differences associated with electricity consumption. The resulting environmental performance therefore remains conditional on both the methanol-production pathway and the onboard electricity-supply scenario.

Consistently, the electricity-emission-factor sensitivity analysis showed that lower-carbon electricity improves the relative sustainability performance of Joule heating. However, no crossover in the aggregated technology ranking was observed over the investigated range of 0.02–0.82 kgCO₂-eq kWh^{−1}. Condensing-steam heating retained the highest aggregate ranking, followed by flue-gas and Joule heating, under every investigated decision-making perspective and aggregation procedure. These results show that the assumed electricity emission factor affects the magnitude of the differences among the configurations but does not alter the overall technology ordering within the investigated emission-factor range and assessment conditions.

3.5.4. Catalyst ageing

A separate limitation concerns transient CO fluctuations and irreversible catalyst ageing. Although the adopted kinetic model captures the steady-state influence of temperature on the competing CO-forming and CO-consuming reaction pathways, it does not predict catalyst service life or irreversible deactivation. Such predictions would require a catalyst-specific, time-dependent deactivation model calibrated against long-duration experiments under representative load variations, thermal cycling, and marine operating conditions.

3.5.5. Electrical-safety limitation

For the Joule-heated configuration, the absence of an additional shell-side process-fluid inventory removes the corresponding DF&EI contributions associated with material inventory, leakage, and pressurised release. The energetic contribution associated with electrical heat generation is nevertheless retained through the additional

exothermic-process factor adopted in the DF&EI calculation. However, the index does not explicitly account for the probability of electrical-equipment failure or marine-specific degradation mechanisms such as water ingress, saline contamination, insulation degradation, tracking, short circuits, or vibration-induced damage. As discussed in Section 2.4.4, these hazards would require a complementary design-specific electrical-safety and reliability assessment.

3.5.6. Mechanical-design limitation

An additional limitation concerns the mechanical detail of the reactor configurations. The reported geometries result from reactor-process and sustainability calculations and should therefore be regarded as preliminary process-design candidates rather than mechanically qualified equipment designs. Detailed shipboard implementation, particularly for elongated configurations such as P27, would require assessment of tube-support spacing, shell and support stresses, thermal expansion, nozzle loads, modal response, vibration-induced fatigue, and ship-specific installation constraints in accordance with applicable classification requirements.

Despite these limitations, the combined thermal, reactor-design, system-integration, and sustainability analyses provide a consistent comparative picture within the assumptions and steady-state design space investigated in this work. Condensing-steam heating achieved the highest aggregate ranking across the examined decision-making perspectives and exhibited favourable steady-state thermal behaviour within the adopted reactor and system boundaries. These findings should not be interpreted as a universal ordering of the heating technologies or as evidence of dynamic superiority, complete mechanical feasibility, or insensitivity to all model and scenario uncertainties. Rather, they identify condensing-steam heating as a promising candidate for subsequent transient modelling, detailed mechanical assessment, and experimental validation, together with further investigation of low-carbon energy pathways, thermal integration, and control strategies for maritime hydrogen-production systems.

4. Conclusions

This study compared Joule-heated, flue-gas-heated, and condensing-steam-heated multitubular MSR reactors integrated with PEMFC systems for maritime auxiliary and propulsion applications. All configurations selected for detailed comparison achieved weighted-average methanol conversions between 99.11% and 99.50%, while the heating mechanism produced marked differences in reactor thermal behaviour and relative sustainability performance. Joule-heated reactors exhibited inlet cold spots of approximately 442–445 K, whereas condensing-steam heating maintained nearly uniform reactor temperatures of approximately 477–478 K. The resulting normalized aggregated sustainability indicators ranged from 0.64 to 0.88 for Joule heating, from 0.87 to 0.96 for flue-gas heating, and from 0.997 to 0.999 for condensing-steam heating. These normalized values express relative performance within the investigated candidate set and should not be interpreted as absolute sustainability levels.

Under the investigated assumptions, condensing-steam heating attained the highest aggregate ranking for both auxiliary and propulsion applications, followed by flue-gas and Joule heating. This ordering was preserved across the Individualist, Egalitarian, Hierarchist, and Equal-weighting perspectives, using both additive and geometrical aggregation, over the discount-rate range of 4–10%, and across the investigated electricity-emission-factor range of 0.02–0.82 kgCO₂-eq kWh^{−1}. Nevertheless, these rankings remain conditional on the adopted reactor and system boundaries, shipboard utility architecture, heat-recovery assumptions, model formulation, membrane-recovery assumption, economic and emission factors, weighting and aggregation procedures, and discrete steady-state operating conditions. They should therefore not be interpreted as a universal ordering of the heating technologies or as evidence of dynamic superiority of condensing-steam heating.

Further work should quantify the sensitivity of the results to membrane recovery, model parameters, utility-price assumptions, and pathway-specific low-carbon fuel scenarios, and should assess whether the present steady-state findings persist under transient operation. This will require coupled models resolving mass and energy accumulation in the gas phase, catalyst bed, and reactor wall; two-phase steam generation, transport, condensation, and condensate drainage; and interactions among the reformer, heat-recovery system, hydrogen-purification unit, PEMFC, energy buffers, and associated control systems. Representative propulsion and auxiliary-load ramps, start-up and shutdown, emergency manoeuvres, wave-induced disturbances, and utility-loss events should be examined with particular attention to response time, temporary hydrogen deficit, CO excursions, catalyst-temperature limits, thermal-gradient evolution, and control stability. Subsequent validation against dynamic experimental data under representative operating conditions will also be required.

CRedit authorship contribution statement

Giuseppe Andriani: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Bojan Grenko:** Writing – original draft, Methodology, Investigation, Formal analysis, Conceptualization. **Gianmaria Pio:** Writing – review & editing, Validation, Software, Methodology. **Chiara Vianello:** Writing – review & editing, Visualization, Supervision. **Ernesto Salzano:** Writing – review & editing, Validation, Supervision, Project administration. **Wiebren de Jong:** Writing – review & editing, Supervision, Resources, Project administration. **Robert van de Ketterij:** Visualization, Validation, Supervision. **Lindert van Biert:** Validation, Supervision, Resources, Project administration, Funding acquisition. **Paolo Mocellin:** Writing – review & editing, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2026.157567>.

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