

Particle swarm optimization for a hybrid freight train powered by hydrogen or ammonia solid oxide fuel cells

Zhang, Yuqi; Yu, Jiacheng; Zhao, Ning; Xu, Zhan; Yan, Yan; Wu, Dawei; Blacktop, Kevin; Tsolakis, Athanasios

DOI:

[10.1016/j.ijhydene.2024.05.347](https://doi.org/10.1016/j.ijhydene.2024.05.347)

License:

Creative Commons: Attribution (CC BY)

Document Version

Publisher's PDF, also known as Version of record

Citation for published version (Harvard):

Zhang, Y, Yu, J, Zhao, N, Xu, Z, Yan, Y, Wu, D, Blacktop, K & Tsolakis, A 2024, 'Particle swarm optimization for a hybrid freight train powered by hydrogen or ammonia solid oxide fuel cells', *International Journal of Hydrogen Energy*, vol. 72, pp. 626-641. <https://doi.org/10.1016/j.ijhydene.2024.05.347>

[Link to publication on Research at Birmingham portal](#)

General rights

Unless a licence is specified above, all rights (including copyright and moral rights) in this document are retained by the authors and/or the copyright holders. The express permission of the copyright holder must be obtained for any use of this material other than for purposes permitted by law.

- Users may freely distribute the URL that is used to identify this publication.
- Users may download and/or print one copy of the publication from the University of Birmingham research portal for the purpose of private study or non-commercial research.
- User may use extracts from the document in line with the concept of 'fair dealing' under the Copyright, Designs and Patents Act 1988 (?)
- Users may not further distribute the material nor use it for the purposes of commercial gain.

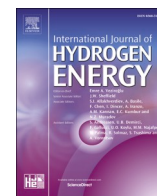
Where a licence is displayed above, please note the terms and conditions of the licence govern your use of this document.

When citing, please reference the published version.

Take down policy

While the University of Birmingham exercises care and attention in making items available there are rare occasions when an item has been uploaded in error or has been deemed to be commercially or otherwise sensitive.

If you believe that this is the case for this document, please contact UBIRA@lists.bham.ac.uk providing details and we will remove access to the work immediately and investigate.



Particle swarm optimization for a hybrid freight train powered by hydrogen or ammonia solid oxide fuel cells

Yuqi Zhang^a, Jiacheng Yu^a, Ning Zhao^b, Zhan Xu^b, Yan Yan^c, Dawei Wu^{a,*}, Kevin Blacktop^d, Athanasios Tsolakis^a

^a Department of Mechanical Engineering, School of Engineering, University of Birmingham, Birmingham, B15 2TT, UK

^b Department of Electric, Electrical and Systems Engineering, School of Engineering, University of Birmingham, Birmingham, B15 2TT, UK

^c School of Mechanical Engineering, Southeast University, Nanjing, 210000, China

^d Birmingham Centre for Railway Research and Education (BCRRE), Birmingham, B15 2TT, UK

ARTICLE INFO

Handling Editor: Fanglin F. Chen

Keywords:

Rail freight

Particle swarm optimization

Solid oxide fuel cell

Hydrogen

Ammonia

ABSTRACT

All diesel-only trains in the UK will be phased out by 2040. Hydrogen and ammonia emerge as alternative zero-carbon fuel for greener railway. Solid Oxide Fuel Cells (SOFCs) provide an alternative prime mover option, which efficiently convert zero-carbon fuels into electricity without emitting nitrogen oxides (NOx), unlike traditional engines. Superior to Proton Exchange Membrane Fuel Cells (PEMFCs) in efficiency, SOFCs fulfil MW-scale power needs and can use ammonia directly. This study investigates innovative strategies for integrating SOFCs into hybrid rail powertrains using hydrogen or ammonia. Utilizing an optimization framework incorporating Particle Swarm Optimization (PSO), the study aims to minimize operational costs while considering capital and replacement expenditures, powertrain performance, and component sizing. The findings suggest that hybrid powertrains based on ammonia-fueled SOFCs may potentially reduce costs by 30% compared to their hydrogen counterparts, albeit requiring additional space for engine compartments. Ammonia-fueled SOFCs trains also exhibit a 5% higher efficiency at End-of-Life (EoL), showing less performance degradation than those powered by hydrogen. The State of Charge (SoC) of the batteries in range of 30–70% for both cases is identified as most cost-effective.

1. Introduction

To meet the 2040 target [1,2] for phasing out diesel trains and achieve Net Zero Greenhouse Gas emissions in transportation, fuel cells are recognized as a crucial technology across automotive, railway, and maritime sectors [3–5]. Hydrogen-powered trains, especially those using Proton Exchange Membrane Fuel Cells (PEMFCs), have shown promise. Alstom's Coradia iLint, the first hydrogen-powered passenger train, has successfully operated on over 1000 km of non-electrified tracks since 2016 [6], while UK's HydroFLEX, a hydrogen-hybrid train with 400 kW PEMFCs, began mainline operations in 2020, achieving speeds of 160 km/h and a 480 km range [7]. Similarly, China introduced its first hydrogen fuel cell hybrid locomotive, capable of hauling a 5000-ton load at speeds up to 80 km/h [8].

However, the preference for high-purity hydrogen makes PEMFCs less ideal for megawatt-scale systems, such as large-capacity and long-distance transport in freight and maritime sectors. Solid Oxide Fuel

Cells (SOFCs) emerge as a superior alternative [9–11], achieving up to 64% energy efficiency—surpassing PEMFCs by 10–20% [12,13]. SOFCs not only offer a 25% efficiency improvement over traditional diesel engines but also considerably reduce NOx and particulate matter emissions [14]. Unlike PEMFCs, which require hydrogen purity above 99.97%, SOFCs can operate on a broad spectrum of fuels, ammonia [13], diesel [14], liquefied methane [15], and bioethanol [16], making them well-suited for megawatt-scale power generation and extensive rail transportation [17].

While SOFC technology presents numerous advantages, challenges related to energy and power management, component sizing, and cost considerations, have limited its industrial adoption. To tackle these challenges in powertrains, numerous optimization strategies have been proposed, primarily categorized into three areas: design, control, and a hybrid approach combining design and control [18].

These efforts focus on optimizing key factors such as capital expenses, operating costs, emissions, and energy consumption, all within

* Corresponding author.

E-mail address: d.wu.1@bham.ac.uk (D. Wu).

<https://doi.org/10.1016/j.ijhydene.2024.05.347>

Received 8 March 2024; Received in revised form 20 May 2024; Accepted 22 May 2024

Available online 31 May 2024

0360-3199/© 2024 The Authors. Published by Elsevier Ltd on behalf of Hydrogen Energy Publications LLC. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

the limits of weight and volume imposed by their transportation applications.

To optimize costs, fuel consumption, emissions, and component sizes in hybrid green systems, Non-dominated Sorting Genetic Algorithm-II (NSGA-II) [19–21], Mixed Integer Linear Programming (MILP) [22, 23], and Particle Swarm Optimization (PSO) [24,25] are the most utilized algorithms [18]. NSGA-II, for instance, has been utilized in a PEMFC-battery ferry [26], effectively determining component sizes to optimize operational expenses and emissions. This approach could reduce life-cycle emissions by 65% versus diesel systems. MILP was employed in a study to model a hybrid PEMFC ferry's long-term operation, focusing on fuel cell, battery costs, and hydrogen fuel expenses. It found that the hydrogen cost proves to be the most significant factor, particularly as the plant approaches the end of its lifetime, with hydrogen consumption experiencing an increase of up to 30% [27]. Soleymani et al. [28] determined the optimal sizes in boats for key components such as the electric motor, internal combustion engine, battery, and generator, employing a constrained PSO approach. This method took into account constraints related to acceleration and speed expectations, potentially achieving a 40% reduction in fuel consumption. These three methods have proven to be efficient for sizing or optimizing of cost-effectiveness. However, PSO demonstrated faster convergence speed than NSGA-II [29,30]. Compared to MILP, PSO achieves better accuracy in meeting the non-linear constraints of the power flow [31]. For large-scale and complex systems, PSO ensures better balance between computational time and satisfactory accuracy.

All three algorithms effectively optimize factors of PEMFC hybrid systems, but PSO stands out for its simplicity and efficiency in transportation applications [32], including marine [33], trains, and vehicles [34,35]. Multi-objective PSO (MOPSO) has been utilized in studies [36, 37] to evaluate the impact of Energy Management System (EMS), train speed, and track slope on component sizing. Adaptive PSO, used in multi-mode trains with PEMFC-battery systems, achieved a 34.9% cost reduction compared to diesel trains [38]. Additionally, PSO's flexible compatibility with other algorithms enhances accuracy of solutions and facilitates the exploration of new technologies and hybrid power systems [33]. A study [21] combined MOPSO with NSGA-II for optimal sizing of solar panels, diesel generators, and batteries in a hybrid tanker, aiming to minimize costs and emissions. Zhu et al. [39] implemented bi-level optimization with Multi-Objective PSO for component sizing and adaptive Equivalent Consumption Minimization Strategy for control, aiming to balance emissions, fuel consumption, and Net Present Cost. This approach surpassed single-level strategies, reducing emissions by 3–7% and costs by 11–14%.

These optimization methods provide solutions of optimizing costs, fuel consumption, and emissions, while considering component sizes. In the optimization of design and control independently, and in combination, PSO is preferred for transportation and hybrid systems due to its simplicity, efficiency, and accuracy in handling multiple objectives.

For SOFC-battery hybrid systems, most optimization studies focus on efficiency and energy management strategies (EMS). A study explored a stochastic power management strategy for a hybrid SOFC and battery auxiliary power unit in heavy-duty vehicles [40]. This strategy aimed to optimize power distribution between the SOFC, auxiliary power unit (APU), and battery, potentially reducing power oscillations in the SOFC, and resulting in over 6% energy savings. Additionally, a 12 kW SOFC-battery model integrated into a modified Nissan Leaf Acenta electric vehicle demonstrated a factor of 5 increase in driving range compared to a standard battery-only vehicle [41]. An adaptive EMS algorithm with a current feedforward strategy has been engineered to efficiently balance power between Li-ion batteries and the SOFC subsystem, ensuring thermal safety and preventing fuel depletion [42].

The integration of SOFCs into power and propulsion systems is valued for their high efficiency and ability to use a variety of fuels [43, 44]. However, critical aspects such as component sizing and cost are not considered in the optimization studies, particularly concerning SOFC

powertrains for MW-scale and long-distance freight trains. But in fact, the increase in the engine room size and weight, due to SOFC applied, leads to higher energy requirement for voyages and dynamic positioning operations [5]. Especially for SOFC-powered railway system, component sizing has impact on rail freight volumes and lift data which serve as essential metrics for assessing freight performance [45]. Consequently, operators might prefer trains with slightly higher lifetime costs if they offer greater capacity.

Additionally, a major limitation in current SOFCs system simulations is the absence of real-time capabilities, which is crucial for accurately capturing SOFC dynamics at various power levels. This limitation is particularly significant for analysing performance of SOFC-hybrid system due to SOFC's very low power transient capabilities, which require that auxiliary power sources, like batteries, have superior rapid adjustment abilities compared to PEMFC-battery systems [46]. Furthermore, although PSO has been applied in various PEMFC-battery transportation applications and other hybrid systems, its use has been limited to identifying reliable and accurate parameters for SOFC [47] or SOFC-gas turbine combined with heat and power system [48]. Despite PSO achieving similar accuracy to the Genetic Algorithm (GA) in system simulations, requiring 187.6 s less time [48], it has yet to be applied in transportation applications for meeting MW-scale power requirements.

Addressing the identified research gaps, this paper proposes the design of an MW-scale hybrid freight train powered by hydrogen or ammonia-based SOFCs. The structure of this paper is organized as follows: Section 1 explains the current situation of optimization for fuel cell hybrid systems and identifies the research gaps in SOFC-hybrid freight optimization simulations. Section 2 describes the drive system, simulation route, and fuel storage. Section 3 presents the real-time SOFC model and the Li-ion battery model. Section 4 outlines the methodology for optimization, considering the limitations of wagon space and cost, using PSO and EMS. It also includes a sensitivity analysis of End-of-Life (EoL) performance and state of charge (SoC) range settings. Section 5 demonstrates the results for hydrogen and ammonia-powered freight, and a 3D design of the SOFC-battery train based on these results is presented.

22. System description

2.1. Selected simulation route and freight train

The selected simulation route spans 318 km from Felixstowe South Gbrf to Hams Hall Gbrf, with six intermediate stops. This study focuses on two specific cases, both utilizing the UK Class 66 freight locomotive, consisting of 20 wagon cars with a total capacity of 1235 tonnes. The drive cycle is based on the daily power request of this freight locomotive, as illustrated in Fig. 1. The orange line represents the time-dependent variation in the locomotive's speed [40], as simulated by the Single Train Simulator software developed by the Birmingham Centre for Railway Research and Education [49]. This software encompasses three core components: the infrastructure model, the vehicle model, and the physics model. The specifics of these components were already integrated into the train simulator [50]. The recordings are captured at 1-s intervals, covering a timeframe of 21,223 s (5.89 h). The route data and freight details were pre-existing in the train simulator, sourced from Network Rail, and previously used in similar simulations [51]. It is assumed that will not differ between the comparative vehicles under investigation.

2.2. Drive-system description

In the development of dual fuel cell drive systems, as depicted in Fig. 2, a diesel-electric power module serves as the foundational model. This approach integrates well-established components such as auxiliaries, traction equipment, and brake resistors, a methodology elaborated upon in Ref. [7]. The innovation in this design lies in its adoption of fuel cell technology for the power plant, comprising a fuel cell power

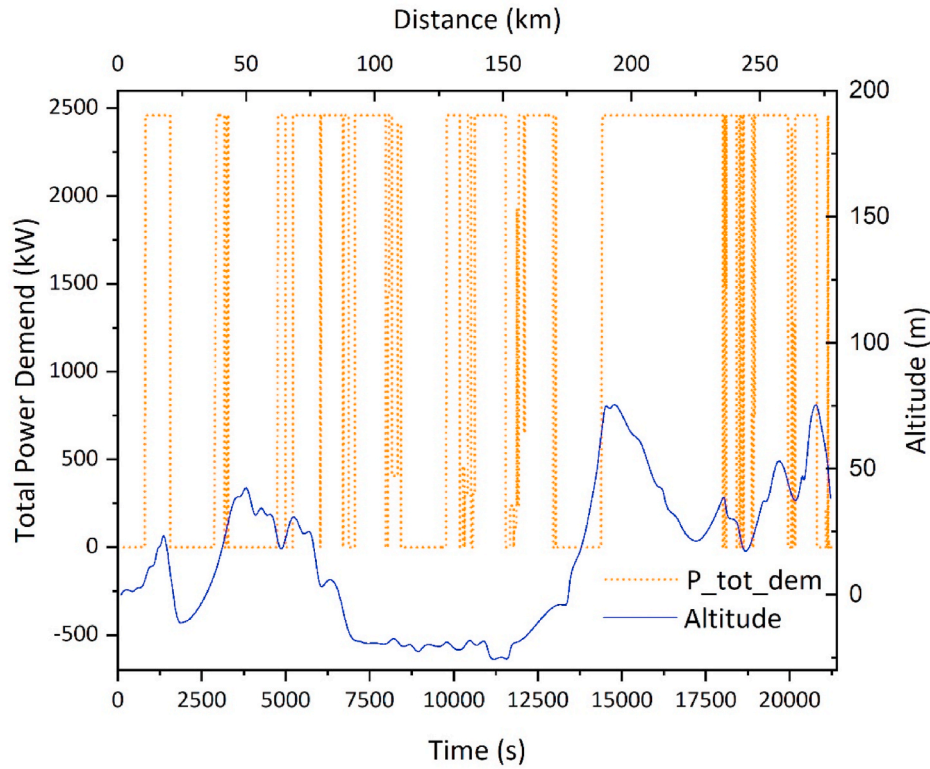


Fig. 1. Line altitude and driving cycles from Felixstowe South Gbrf to Hams Hall Gbrf [52].

system alongside an energy storage system, both interfacing with the Direct Current (DC) bus through DC-to-DC converters.

Hydrogen-powered drivetrain configuration, shown in Fig. 2(a), includes a preheating process for hydrogen and air before entry into the fuel cell, enhancing efficiency as outlined in Refs. [53,54]. The SOFC stack processes fuel into power and exhaust gases, employing counter-flow heat exchangers to preheat incoming fuel and air, ensuring optimal operational temperatures.

Furthermore, three operational modes—direct ammonia, external decomposition, and autothermal decomposition—have been implemented in ammonia-fueled SOFC stacks [55], capable of delivering 1 kW of power output with an electrical efficiency of 52%. These modes, however, remain underexplored for transportation applications. In Fig. 2(b), the ammonia fuel cell power system uses commercial ammonia cracking technology to convert ammonia into hydrogen via high temperature thermocatalytic reforming, with operational temperatures around 1073 K [56]. This process achieves approximately 89.7% system efficiency. A separation membrane ensures the SOFCs supplied with high-purity hydrogen, as corroborated by Ref. [56].

2.3. Fuel and storage

Tables 1 and 2 present the geometric parameters for the SOFC, battery, hydrogen tank, and ammonia tank. To comply with the operational requirements of freight trains, which include continuous operation for over 6 h daily, the drive systems and storage configurations are designed to eliminate the need for refueling during a single trip. Compressed gas hydrogen storage technology at 350 bar, as highlighted in previous research [4,57], is widely used in drive systems. For rail applications, 350 bar storage tanks are preferred due to their 17.6% less cost compared to 700 bar tanks [58].

In the case of ammonia-fueled powertrains, ISO containers are selected for ammonia storage. Their suitability for long-distance transport and low leakage rates have been confirmed by ISO standards and leakage safety inspections [66]. These containers operate at pressures of

8–22 bar and temperatures ranging from 233 to 333 K. Cost analyses by Ref. [67] show that ammonia storage costs are £2.49/kg and £0.56/kg for small-scale and large-scale storage, respectively. Liquefied ammonia, containing 50% more hydrogen by volume than liquid hydrogen, is identified as a safe, efficient, and cost-effective hydrogen storage medium [68].

3. Physical models of components and validations

As described in the system overview, the freight train employs a hybrid power generation system that integrates SOFCs and batteries. This section presents the development and validation of models for the primary power source.

3.1. SOFC model and validation

The model calculates current-voltage characteristics and fuel consumption across various power loads. It incorporates an electrochemical model that delineates the relationship between cell voltage (V_{cell}) and irreversible overvoltage, as formulated in Eq. (1)

$$V = E - \eta_{con,a} - \eta_{con,c} - \eta_{act,a} - \eta_{act,c} - \eta_{ohm} \quad (1)$$

Where E represents the local Nernst potential, η_{con} refers concentration overvoltage, η_{act} denotes activation overvoltage, and η_{ohm} signifies ohmic overvoltage. The reversible voltage E is detailed in Eq. (2)

$$E = 1.253V - \left(2.45167 \times \frac{10^{-4}V}{K} \right) \cdot T_{cell} - \frac{RT}{4F} \ln \left(\frac{P_{H_2O}^2}{P_{H_2}^2 \cdot P_{O_2}} \right) \quad (2)$$

The activation overvoltage, originating from the necessary activation for charge transfer at electrodes, is defined by the Butler-Volmer equation. This is articulated in Eq. (3), with the exchange current density being influenced by the microstructure of the electrode and the operating conditions, as elaborated in Eqs. (3)–(6) [69].

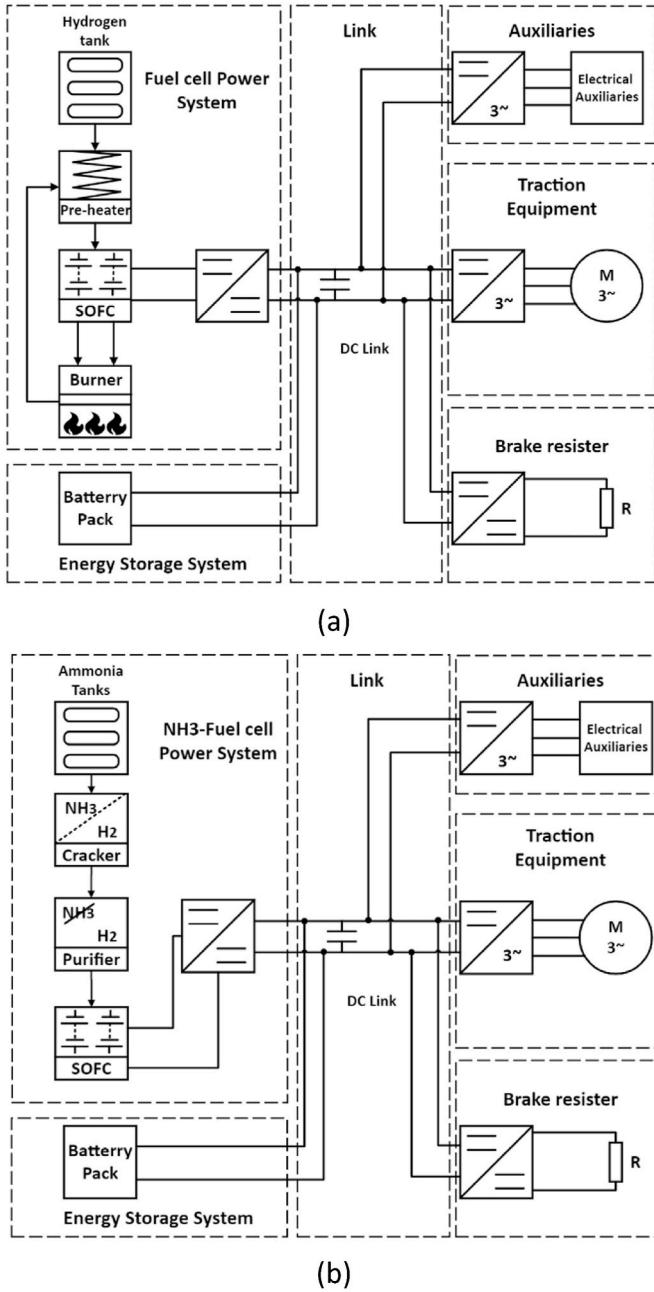


Fig. 2. Power-module drive-system diagrams for two different trains. a) Hydrogen-SOFC train, b) Ammonia-SOFC train.

Table 1
Geometry parameters and economic data of SOFC and battery. [[59–61]].

	Model	Width (m)	Length (m)	Height (m)
SOFC	3 kW	0.19	0.23	0.28
Battery	25 kWh	0.6	0.6	1.422

Table 2
Geometry parameters and economic features of hydrogen and ammonia tank. [[62–65]].

Tank fuel	LHV (MJ/kg)	Pressure (bar)	Diameter (m)	Width (m)	Length (m)	Height (m)	Capacity (kg)
Hydrogen	120	350	0.415	–	2.1	–	5
Ammonia	43.1	22	–	2.44	6.058	2.59	1245.74

$$\eta_{act,n} = \frac{RT}{F} \sin h^{-1} \left(\frac{J}{2J_{0,n}} \right) = \frac{RT}{F} \ln \left[\frac{J}{2J_{0,n}} + \sqrt{\frac{J^2}{2J_{0,n}^2} + 1} \right], n = a, c \quad (3)$$

$$J = J_0 \left[\exp \left(\frac{a_z F \eta_{act}}{RT} \right) - \exp \left(- \frac{(1-a) z F \eta_{act}}{RT} \right) \right] \quad (4)$$

$$J_{0,a} = (1.3448E + 10) \times \left(\frac{P_{H_2}}{P} \right) \left(\frac{P_{H_2O}}{P} \right) \exp \left(- \frac{E_{act,a}}{RT} \right) \quad (5)$$

$$J_{0,c} = (2.051E + 9) \times \left(\frac{P_{O_2}}{P} \right)^{0.25} \exp \left(- \frac{E_{act,c}}{RT} \right) \quad (6)$$

The concentration overvoltage results from the concentration gradient of reactants or products in the bulk electrolyte and on the electrode surface. This is expressed in Eq. (6).

$$\eta_{conc} = \frac{RT_{cell}}{2F} \ln \left(\frac{1 + \frac{RT_{cell} \cdot c_a \cdot J}{2F \cdot D_{eff, An} \cdot P_{H_2O}^0}}{1 - \frac{RT_{cell} \cdot l_c \cdot J}{2F \cdot D_{eff, An} \cdot P_{H_2}^0}} \right) + \frac{RT_{cell}}{4F} \ln \left[\frac{P_{O_2}^0}{\frac{P_c}{\delta_{O_2}} - \left(\frac{P_c}{\delta_{O_2}} - P_{O_2}^0 \right) \exp \left(\frac{RT_{cell} \cdot l_c \cdot J \cdot \delta_{O_2}}{2F \cdot D_{eff, Cat} \cdot P_c} \right)} \right] \quad (7)$$

The ohmic overvoltage, η_{ohm} , is results from ohmic resistance of electrolyte, anode, and cathode. Typically, it is the resistance encountered by oxygen ions moving through the electrolyte that predominantly contributes to the resistance, symbolized as r . Thus, the ohmic overvoltage can be simplified in the following manner.

$$\eta_{ohm} = (r_e l_e + r_c l_c + r_a l_a + r_{contact} l_{contact}) i \quad (8)$$

The efficiency of SOFC is given by Eq. (9):

$$\eta_{cell} = \frac{P_e}{Q_{in}} = \frac{\int I \cdot V_{cell} dA}{\dot{m}_{f,in} \cdot \Delta h_{f,in}} = \eta_{rev} \cdot \eta_v \cdot \eta_u \quad (9)$$

$\dot{m}_{f,in}$ represents the instantaneous hydrogen consumption rate of the SOFC stack, and it can be formulated as a function of the operating current, I , in the following way:

$$\dot{m}_{f,in} = \frac{n_{cell} \cdot I \cdot M_{H_2}}{2F} \quad (10)$$

Table 3 summarizes the relevant operating and geometric parameters used in the experiment.

Table 3
The main parameters for the model of SOFC and validation [69,70].

Parameters	Unit	Values
P_{H_2}	H_2 pressure at anode	bar
P_{H_2O}	H_2O pressure at anode	bar
P_{O_2}	O_2 pressure at cathode	bar
P_c	Operating cathode pressure	bar
l_a	Anode thickness	m
l_c	Cathode thickness	m
l_e	Electrolyte thickness	m
ϵ	Electrode porosity	–
ζ	Electrode tortuosity	–
$E_{act,a}$	Activation energy for anode	J/mol
$E_{act,c}$	Activation energy for cathode	J/mol

Fig. 3 displays a comparison of the SOFC performance from both simulation results and experimental data across different temperatures. The notable congruence between the simulation and the experimental results indicates the effectiveness of the current SOFC model in accurately predicting SOFC performance.

3.2. Li-ion battery model and validation

In this study, the battery technology utilized is Lithium-titanate-oxide (LTO). Distinct from other Lithium-ion (LiB) materials, LTO not only offers a lower nominal voltage and energy density but also incorporates spinel as an effective anode material. This attribute is especially beneficial in high-power electric mobility sectors such as trains, ships, and heavy-duty vehicles, where the ability to deliver instantaneous power for swift acceleration is essential [71].

In line with the energy management requirements, the instantaneous power demand is split between the battery and the fuel cell. Therefore, the variable power exchanges at each point in time are defined by Eq. (10a).

$$P_{Batt}(t) = P_{dem}^{tot}(t) - P_{FC}(t) \quad (10a)$$

Where, $P_{dem}^{tot}(t)$ is the total instantaneous power demand for the locomotive. The $P_{Batt}(t)$ can have a positive, negative, or zero or value. A positive $P_{Batt}(t)$ signifies the battery is discharging, whereas a negative value indicates charging. When $P_{Batt}(t)$ is zero, it means the battery is idle. The SOC of the battery at any given instant is calculated based on its SOC at the previous time step ($t - \Delta t$). Following this mathematical expression [37]:

$$SoC_{Batt}(t) = SoC_{Batt}(t - \Delta t) - \eta_{Batt} \frac{P_{Batt}(t)}{Q_{Batt}^{rated}} \Delta t \quad (11)$$

Where, η_{Batt} denotes the efficiency of the battery during charging or discharging. The computation of this efficiency is as follows:

$$\eta_{Batt} = \begin{cases} \frac{1}{\eta_{chg}}, P_{Batt}(t) \leq 0 \\ \eta_{dis}, P_{Batt}(t) > 0 \end{cases} \quad (12)$$

The η_{chg} and η_{dis} are the charging and discharging efficiencies of the battery, Q_{Batt}^{rated} is the battery capacity, and Δt is the small increment in time.

4. Optimization model

Detailed here are the EMS strategies for distributing power between

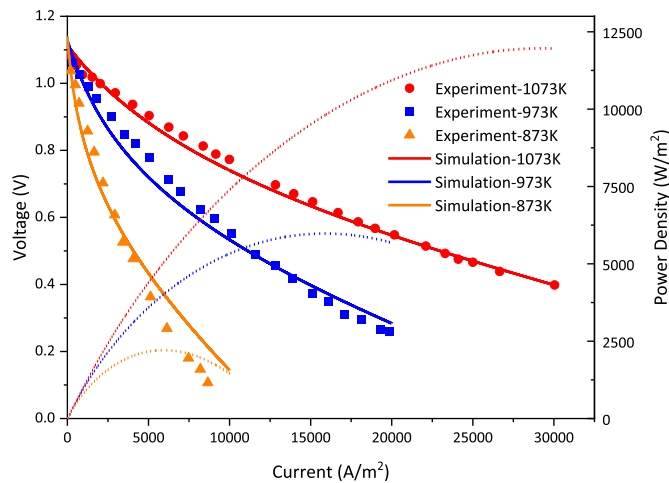


Fig. 3. Validation of SOFC electrochemical model.

the SOFCs and batteries. These strategies aim to maximize efficiency and minimize fuel consumption. On the financial side, effective design considerations such as cost modeling, component sizing, and the PSO are outlined to achieve a balance between performance and cost-effectiveness. Additionally, key sensitivity factors, including SoC, startup time, and EoL performance are discussed to provide a thorough understanding of the system's performance parameters.

4.1. Sizing

4.1.1. Particle swarm optimization

PSO is an algorithm inspired by the social behavior of birds and fish, such as flocking and schooling. Chosen for its suitability in railway applications, PSO is noted for its simplicity, cost-effectiveness, robustness, accuracy, and fast convergence. In this study, PSO is employed to identify the optimal sizes of SOFC stacks and batteries to minimize the levelized cost of electricity. Each solution in PSO, referred to as a 'particle,' represents the sizes of the SOFC and battery. The EMS is incorporated as a supporting subroutine within the main PSO algorithm. Fig. 5 presents a flowchart of the comprehensive solution strategy.

Particles that exceed specified volume limits or deviate from the optimal state of charge range are penalized. In this study, 'freight train' refers to flatbed wagons carrying ISO standard shipping containers, pulled by a Class 66 locomotive [72]. Key factors such as rail freight volumes and lift data are essential for assessing freight performance. Operators might opt for trains with higher lifetime costs if they offer increased capacity. To preserve cargo capacity, the combined volume of all powertrain components, including fuel cell stacks, batteries, and tanks, should ideally not exceed that of a single Class 66 locomotive.

The PSO algorithm begins with an initial group of particles, each assigned random values and velocity vectors, and a population size of 20. The range of values for each particle is derived from the minimum and maximum numbers of SOFCs and batteries that can feasibly be installed on the train, considering the available car space and adhering to the UK gauging criterion. This approach balances the need for adequate power to complete routes with the constraint of available train space.

4.1.2. Weighting factor selection

The movement of particles within the search space is influenced by their velocity, each particle's best previous position, and the best previous position achieved globally. The position corresponding to a particle's optimal fitness value is termed ' p_{best} ', while ' g_{best} ' refers to the position associated with the highest fitness value across the entire population of solutions. The velocity vectors are crucial in guiding the particles' trajectories in the search space. The relevant formulas are outlined as follows:

$$v_i(t+1) = \omega v_i(t) + c_1 r_1 (P_i(t) - x_i(t)) + c_2 r_2 (g(t) - x_i(t)) \quad (13)$$

$$x_i(t+1) = x_i(t) + v_i(t+1) \quad (14)$$

Where v_i is the velocity of the particle. ω is the inertia weight, which represents the degree to which the particles are influenced by the inertia of their motion at the previous moment and can be used to optimize the performance of the PSO. c_1 and c_2 are the individual learning factors and group learning factors respectively, which are used to control the dependence of individual velocity changes on the positions of p_{best} and g_{best} , which are generally set to random numbers within 0~2. r_1 and r_2 are generally set to random numbers within 0~1, which are used to maintain the diversity of the particle swarm, t is the number of current iterations.

Once the algorithm has performed a higher number of algorithms, there is confidence that the particles have begun to converge on the optimal point, so it is appropriate for the velocity of the particle to increase. This avoids the challenges associated with slow convergence if a

low learning factor is chosen and mitigates the risk of the particles converging on a local minimum rather than the global minimum if a high learning factor is selected. The impact of the current velocity on the next generation's velocity can be regulated by adjusting the inertia weight ω . A larger ω enhances global exploration of particles, whereas a smaller ω favors local exploitation. In line with the inertia weight adjustment strategy, both constant and time-varying inertia weights are commonly employed in the fitness function.

To circumvent falling into a local optimum, a non-linear adaptive inertia weight is applied to this study. A nonlinearity ω based on the number of iterations could enhance ω when the algorithm falls into a locally optimal solution, providing a better balance between local and global search capabilities. A non-linear adaptive inertia weight is also evaluated and is expressed as [73]:

$$\omega_3 = \omega_{\min} + (\omega_{\max} - \omega_{\min}) * \cos\left(\frac{\pi}{2 * \left(\frac{k}{iter_{\max}}\right)^{\frac{1}{2}}}\right) \quad (15)$$

4.1.3. Penalty

As illustrated in Fig. 4, penalty functions play a pivotal role in the PSO process, adeptly removing constraints and imposing penalties on the objective function when the battery's SoC exceeds predefined limits. Achieving a delicate balance between feasibility and optimization poses a challenge for penalty functions. In the context of Genetic Algorithms (GAs), research [74] suggests that an excessively high penalty compels

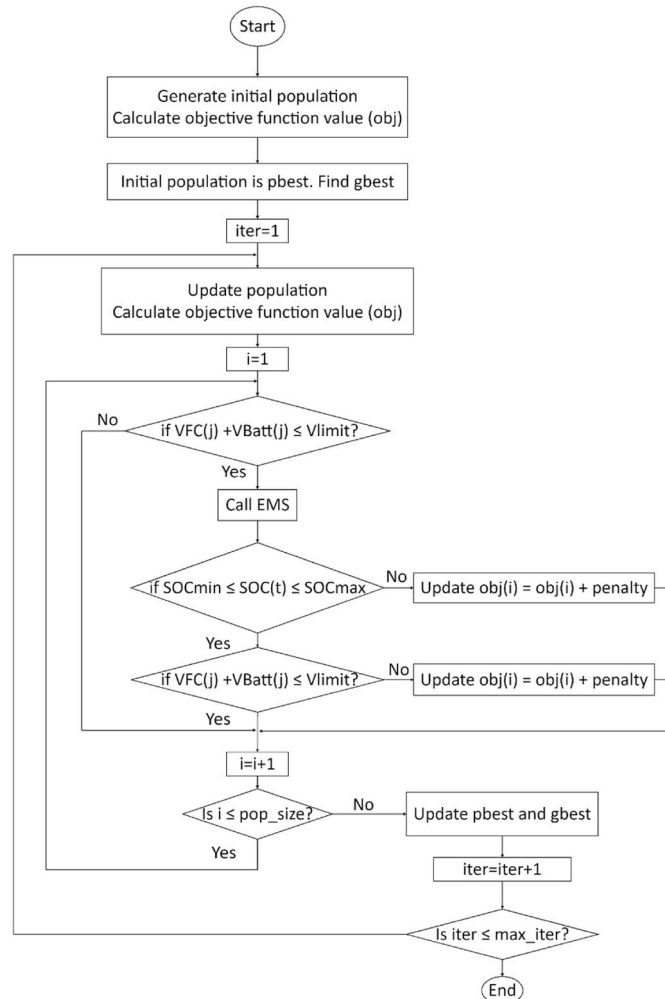


Fig. 4. Flowchart of particle swarm algorithm.

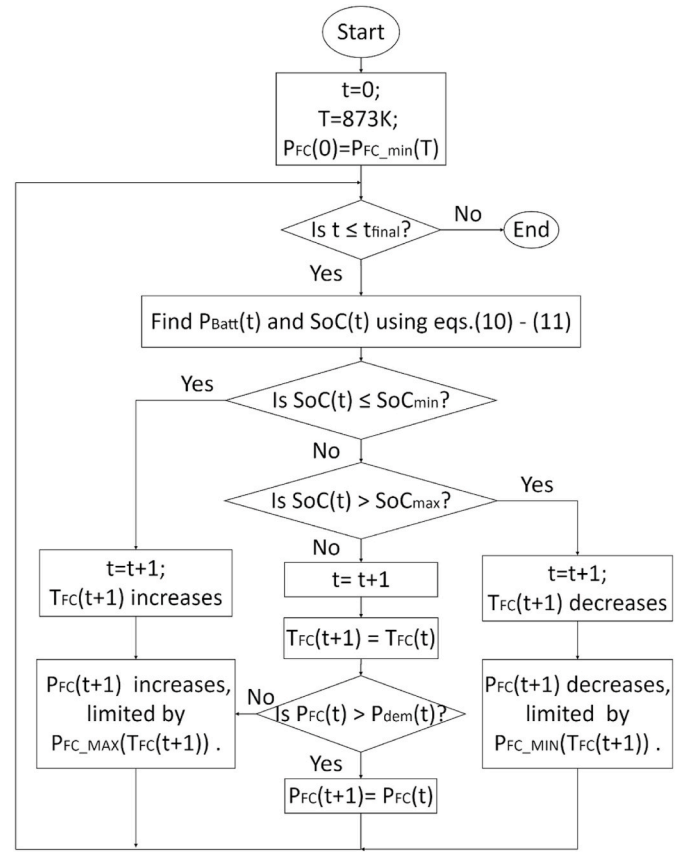


Fig. 5. Flowchart of energy management strategy.

the GA to prioritize feasibility over optimality. Conversely, a too-small penalty diminishes the emphasis on feasibility, risking a failure to converge.

This study meticulously examines both constant and variable penalty approaches. While the constant penalty method is recognized as less effective for intricate problems, its simplicity lends itself to easy application. This approach involves applying a fixed penalty upon a violation. In contrast, variable penalty functions adjust penalties proportionally to the objective function value, contingent on the extent to which the SoC exceeds its defined boundary.

For the constant penalty function:

$$F_c(x) = f(x) + C \quad (16)$$

$$C = \begin{cases} 0, & \text{if } \text{SoC}(t) > \text{SoC}_{\max} \text{ or } \text{SoC}(t) > \text{SoC}_{\min} \\ \sum_{t=0}^{t_{\text{final}}} k_{c_penalty}, & (m = \min, \max) \text{ otherwise} \end{cases} \quad (17)$$

4.2. Objective functions and constraints

After the algorithm is initialized and the initial particle set is generated, a fitness value is assigned to each particle. This value is determined by the objective function that needs optimization and is mathematically formulated in Eq. (18)

$$f(x) = \frac{C_{inv,a} + C_{rep,a} + C_{O\&M,a}}{E_{electricity}} \quad (18)$$

Where $C_{inv,a}$ represents the amortized annual capital cost, a crucial factor for manufacturers contemplating significant investments in fuel cells, batteries, and auxiliary equipment. Integrating capital costs into the objective function allows manufacturers to efficiently assess and address potential project risks, including return on investment and payback

periods. This consideration is particularly vital considering the higher cost of SOFCs compared to other fuel cell types and conventional powertrain solutions. The estimation of $C_{inv,a}$ is as follows [51]:

$$C_{inv,a} = \frac{r(Cap)}{1 - (1 + r)^{-n}} \quad (19)$$

In this equation, r stands for the annual interest rate, Cap represents the capital cost, and ‘ n ’ refers to the loan’s duration in years. Given the substantial capital costs, financing through a loan is necessary. The loan period aligns with the approximate 25-year lifespan of a locomotive engine. An annual interest rate of 2.5% is applied. The capital cost Cap is further defined in Eq. (20)

$$Cap = C_{FC} + C_{Batt} + C_{fuel-25} + C_{cracker} \quad (20)$$

Here, C_{FC} , C_{Batt} , and $C_{cracker}$ represent the capital costs of the SOFC stacks, battery, and ammonia cracker, respectively, as detailed in Table 4. The fuel costs, denoted as C_{fuel_j} , are incorporated into the function, given their significance to operators. Additionally, fuel consumption correlates with the volume of the storage tanks, which directly impacts the cargo capacity of a freight train.

The fuel costs for the two considered drive systems, denoted as (C_{fuel_j}), are computed using Eq. (23). It is assumed that the fuel price, P_{fuel} , varies annually at a rate similar to historical trends, with the fuel price in the j -th year, $P_{fuel}(j)$, calculated according to Eq. (24). Reflecting the 25-year operational lifespan of a freight train’s locomotive, the fuel prices for the five trains are estimated over this period. Assuming that each train uses $M(fuel)_{powertrain}$ fuel annually as planned, the total fuel cost over 25 years for both hydrogen and ammonia, $C_{fuel-25}$, is derived using Eq. (23) [38].

$$C_{fuel_j} = P_{fuel_j} \times M(fuel)_{Power-Plant} \quad (21)$$

$$P_{fuel}(j) = P_{fuel}(py) \times (1 + j \times r) \quad (22)$$

$$C_{fuel-25} = M(fuel)_{Powertrain} \times \sum_{j=1}^{25} P_{fuel}(j) \quad (23)$$

Typically, all equipment has a predetermined life cycle and requires replacement upon reaching its end. In this project, the replacement costs for key components, including the fuel cell prime mover C_{FCrep} , ammonia cracker $C_{CRACKER}$, and battery, are taken into account. The combined costs of these components are represented as C_{rep} in Eq. (24).

$$C_{rep} = C_{FCrep} + C_{CRACKER} + C_{BRep} \quad (24)$$

$$C_{CRACKER} = \frac{\text{Installed CAPEX of cracker}}{\text{Maximum traction power}} \quad (25)$$

The Installed CAPEX of cracker is linearly related to the hourly hydrogen consumption [56]. This correlation is reformulated into a new metric, as specified in Eq. (27). The battery pack, subject to degradation, necessitates replacement over time. With each charging and discharging cycle, the battery’s capacity gradually diminishes. Once its maximum capacity drops to approximately 75%, the battery is considered to have failed. The associated replacement cost for the battery is presented as follows [38]:

$$C_{BPrep} = C_{BP} \times \left(\frac{\int \frac{P_{BP,disch}}{Cap_{BP}}}{DOD_{lifespan}} - 1 \right) \quad (26)$$

$P_{BP,disch}$ is the power of discharging, Cap_{BP} is the battery capacity, and $DOD_{lifespan}$ is the depth of discharge [31].

The annualized replacement cost ($C_{rep,a}$) is defined as:

$$C_{rep,a} = \frac{i \cdot (1 + i)^n}{(1 + i)^n - 1} \cdot \frac{C_{rep}}{(1 + i)^t} \quad (27)$$

where i is the interesting rate, n is the loan years, and t is the lifespan of the facility.

The objective function is also the levelized cost of electricity (LCOE), which is calculated as:

$$LCOE = \frac{\text{Total Costs (£)}}{\text{Annual Electricity Production (kWh)}} = \frac{C_{inv,a} + C_{rep,a} + C_{O\&M,a}}{E_{electricity}} \quad (28)$$

4.3. Energy management strategy

The instantaneous power demand of the fuel cell stack and battery varies in response to the train’s drive cycle. The EMS operates throughout the cycle with the aim of determining the power allocation between energy sources to meet the train’s power requirements. Fig. 5 illustrates the EMS for the hydrogen SOFC train. The power management strategy is executed based on the battery’s state of charge (SoC) and the instantaneous power demand. The primary control rule dictates that if $P_{FC}(t)$ is less than $P_{dem}^{tot}(t)$, the battery operates in discharging mode to provide additional power for the train. Charging of the battery occurs when the $P_{FC}(t)$ exceeds $P_{dem}^{tot}(t)$. The SoC of the battery is a pivotal parameter governing SOFC performance level. The specifics of start-up and operating control are outlined below.

To minimize the energy consumption of the system’s heating and to avoid the SOFC operating at high temperatures for extended periods, which enhances its longevity, the SOFC’s operational temperature is varied according to the SoC. It initially starts at a minimum power output at 837 K. The $P_{Batt}(t)$ and $SoC_{Batt}(t)$ could be calculated using Eqs (10) and (11). If the $SoC(t)$ falls below a certain minimum, it indicates that more power is required from the SOFC not only meet the power demand from the train’s DC link but also to charge the battery. Therefore, the SOFC’s operating temperature ($T(t + 1)$) is increased to enhance its maximum power output limit. This increase is based on the principle that a higher operating temperature usually results in a higher power output, as described in the physical model of the SOFC in Section 3. The SOFC power output ($P_{FC}(t)$) is also increased by elevating the mass flow rate to meet the power requirements. If the $SoC_{Batt}(t)$ exceeds the maximum limit, the operating temperature and power output of the SOFC are reduced to allow the battery to discharge and maintain the SoC within the specified limits. If none of these conditions are met, the power output and operating temperature of the SOFC will remain unchanged.

Table 4
CAPEX, O&M, and REPLEX.

System	CAPEX						O&M	REPLEX
	SOFC	Battery	Cracker	Installation	Fuel	Fuel tank		
	£/kW	£/kWh	£/kW, ton H ₂ /hr	£/kW	£/kg	£/m ³	£/kW	£/kW·10yrs
H2-SOFC	4150.00 [60]	277.00 [75]	–	973.90 [60]	1.82 [62]	10,043.00 [76]	228.25 [60]	1779.11 [60]
NH3-SOFC	4150.00 [60]	277.00 [75]	823.92, 0.075 [56]	1164.00 [60]	0.11 [64]	1802.70 [77]	432.00 [78]	3366.74 [60]

4.4. Sensitive factors

4.4.1. State of charge

As outlined in the EMS documentation, the power output of SOFC is constrained by the SoC settings, which influence fuel consumption—a critical factor for tank and component sizing in this study. Additionally, the adjustment of SoC setting is closely linked to the degradation mechanisms and lifetime of Lithium-titanate-oxide (LTO). These factors are of paramount importance for both manufacturers and customers, as they directly impact the overall system's profitability.

A clear relationship between the depths of discharge and the degradation level is evident. After 2400 equivalent full cycles, the mechanical stress during lithiation and delithiation leads to loss of active material on the positive electrode, resulting in capacity decrease and inner resistance increase. The SoC range of 0–100% has 10–15% greater reduction in capacity and around a 20% increase in inner resistance compared to the 10–50% and 5–95% SoC ranges. Furthermore, the SoC range of 5–95% undergoes the strongest degradation among other settings [79]. Therefore, it is crucial to acknowledge that the adjustment of SoC levels, whether too high or too low, can significantly affect system performance and lifespan. Consequently, maintaining optimal SoC levels through careful management is essential.

In hybrid powertrain systems, integrating battery and fuel cell technologies, the specific limit of battery SoC is not rigidly defined, especially for SOFC, which is not a fully mature technology in heavy-duty powertrain. However, the role of SoC within the EMS is pivotal, as it dictates the proportional utilization of battery and fuel cell resources. To effectively navigate these complexities, a comprehensive simulation has been conducted, encompassing seven distinct SoC ranges (0–100%, 10–90%, 20–80%, 30–70%, 20–50%, 50–80%). This simulation is designed to pinpoint a SoC configuration that optimally balances energy efficiency with economic viability, thereby advancing the capabilities of these sophisticated hybrid powertrain systems.

4.4.2. Startup

During the start-up phase, the SOFC must be heated to its operational temperature range, between 873 K and 1073 K, to commence electricity generation. This is achieved through two prevalent methods. The first involves connecting the bipolar plate's heating elements to an electrical power source. The second method preheats the cathode air using an electric burner before passing it through the stack. Properly adjusting the inlet pressure is critical during the heating process, as flow resistance within the stack tends to increase with temperature. Both methods necessitate a controlled heating rate to avoid exceeding the SOFC stack's thermal stress limits and require a comparable amount of heating energy. Reducing the thermal mass of the hot components is beneficial in shortening both start-up and cool-down durations. Currently, a cold-start SOFC typically takes between 12 and 24 h to start up, while a hot start requires approximately 0.1–0.2 h [46]. For the shutdown process, the stacks are cooled down gradually, typically by passing air over the cathode of the SOFC stack.

Based on estimations [80] and experiments [81], it's observed that the heat loss during the SOFC's initial warm-up phase, from atmospheric temperature to its high operating temperature, is significantly 20% greater than maintaining the cell at the high temperature. From a perspective of long-term start-up and heat loss considerations, the hot standby mode becomes a more viable option. The electricity generated during hot standby can be stored in an auxiliary battery or fed into the grid network, functioning as a small power plant. This capability presents significant advantages for the SOFC railway system. Therefore, the SOFC is set to operate in hot standby mode throughout the entire process. The SOFC is heated to 873 K before the train sets off. The temperature increases when higher output power is demanded; otherwise, it remains at 873 K. For heat-up, as described in the drive-system section, the operating temperature of the SOFC is maintained by the heat energy from its chemical reaction's production steam [82,83]. If there's a

sudden increase in power demand and SOFC's own heat production is insufficient, burning hydrogen from the tank would serve as an additional heat source.

4.4.3. End of life

In high-temperature fuel cell applications, especially with SOFCs, operational lifespan is a crucial factor influenced by various degradation mechanisms. This aspect is of paramount importance to manufacturers and end-users, given the substantial investment costs. Degradation, mainly marked by the decrease in cell active area, significantly impacts power output. According to the U.S. Department of Energy's (DOE) Fuel Cell Technologies Office, a degradation rate of 0.2% per 1000 h is considered acceptable [84]. Simulations aiming to replicate long-term performance have shown that SOFC stacks can maintain stable power output by adjusting fuel flow. This approach effectively counters the effects of voltage degradation and prevents fuel starvation. For battery systems, the end-of-life is typically defined by a capacity reduction to 80%. While simulations often presume ideal operational conditions, practical applications require designs that ensure sustained performance, even in states of degradation. This is essential to meet real-world contractual obligations for system reliability at the end of their operational lifespan.

5. Results and discussion

In this section, simulations are conducted to assess the performance of the proposed SOFC train using two different fuels: hydrogen and ammonia, as detailed in the 'drive-system' section. The design approach is constrained by space limitations with the objective of minimizing LCOE. This section introduces and analyzes the outcomes of a sensitivity analysis concerning the PSO weighting factors, the battery's state of charge, and the EoL of the SOFC and battery. Following this, the section details the design of a solution incorporating the best-identified parameters, discusses the system's performance, and presents the corresponding results.

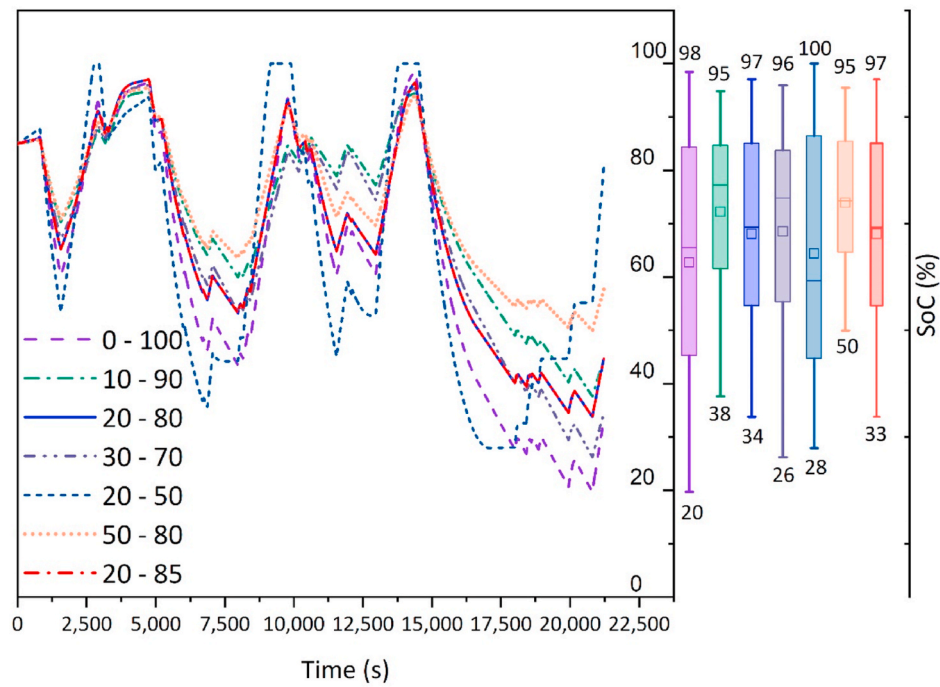
5.1. Sensitive analysis results

5.1.1. State of charge

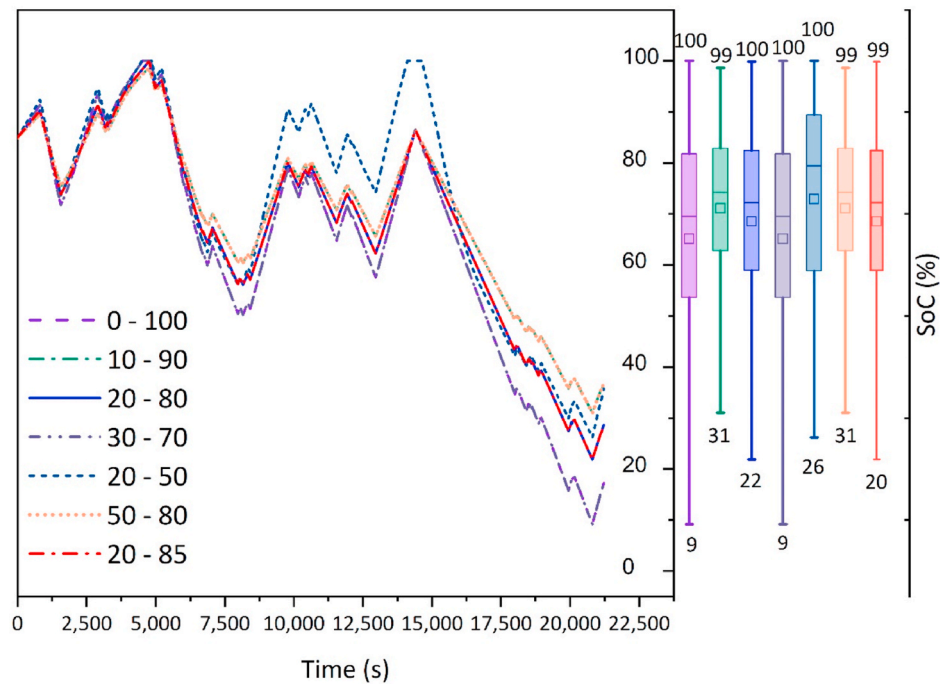
The results from the simulations, as presented in Fig. 6, reveal that actual SoC exceeded the pre-set values, attributed to the employment of a simplistic penalty function within the PSO algorithm, which exhibited tolerance for higher penalties. Nevertheless, a substantial 85% of the data conformed to the expected range. This finding suggests that for stringent SoC regulation, a refined penalty function—adaptive to iterative changes and previous SoC readings—is requisite to enhance accuracy.

Observations from the temporal SoC progression indicate homogeneity in fluctuations up to 17,500 s. Post this juncture, only the SoC ranges of 20–50% demonstrated a reversion to its initial values in the case of hydrogen systems, unlike the others which persisted in a declining trend. This is attributable to the comparative power outputs of the fuel cell and battery systems (Fig. 7), which suggests the charging requirement at the station could be reduced when the output power of the two remains equivalent. However, in the ammonia system, no SoC range returned to its initial setting. The ammonia system, due to lower powertrain efficiency from ammonia cracking and the high cost of SOFCs, requires more batteries. Consequently, there are insufficient fuel cells to recharge the battery to its original SoC. This consideration becomes crucial in driving scenarios requiring batteries to be recharged to their full capacity.

The sensitivity analysis of SoC for both systems reveals that the 0–100% and 20–50% range is detrimental to battery lifespan, leading to extreme SoC levels. The 30–70% range is the most cost-effective due to minimal fuel consumption. The 50–80% and 20–80% ranges are favorable for battery lifespan, as most SoCs in these scenarios hover around



(a)



(b)

Fig. 6. State of charge variations over time in SOFC train with different SoC range settings: a) H₂-SOFC SoC; b) NH₃-SOFC.

75–80%.

Despite variations in SOFC and battery sizes, hydrogen consumption is more influenced by the number of SOFCs than by the number of batteries, indicating that SOFCs have a greater impact on overall costs. Balancing performance, cost, and longevity may necessitate a narrower SoC range, particularly around 70–80%. Determining the optimal SoC range will require further analysis and enhancements in control

strategies. Current studies commonly explore SoC settings ranging from 20% to 85%, but these may not be the most economical ranges.

5.1.2. EoL of SOFC and battery

In the application of EoL mode to fuel cells and batteries, this configuration necessitates increased resource usage due to the diminished efficiency of the fuel cells and the lower capacity of the batteries.

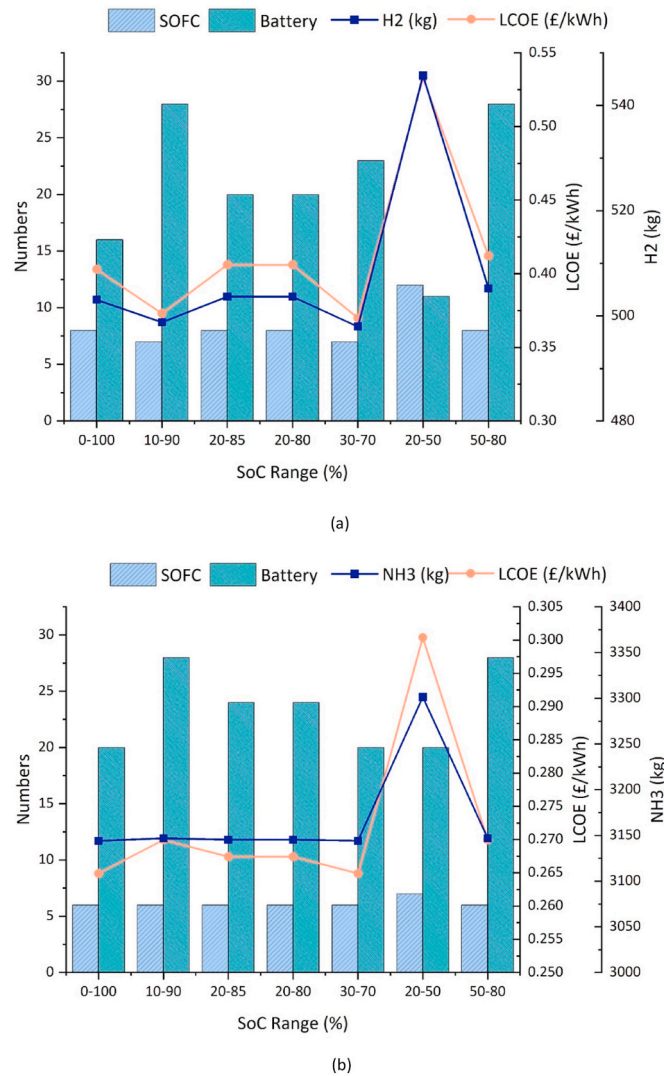


Fig. 7. Number of SOFCs and battery, LCOE, and fuel consumption for SOFC train across different SoC range settings: a) H2-SOFC SoC; b) NH3-SOFC.

Fig. 8 displays the change in battery SoC from BoL to EoL. At BoL, the battery SoC predominantly hovers around 68%, but this figure drops to approximately 53% at EoL, indicating a significant capacity reduction. However, despite this decrease, the SoC range at EoL only marginally expands in ammonia-based systems, with the primary SoC shifts being minimal. This implies that, overall, battery performance remains relatively stable over their lifespan.

As depicted in Fig. 8(b), the data primarily clusters at the highest and lowest levels, correlating to frequent phases of deceleration and acceleration, which correspond to the lowest and highest power demands, respectively. Additionally, SOFCs exhibit a less pronounced reduction in efficiency when using ammonia as opposed to hydrogen. The average efficiency of SOFCs decreases by 23% in systems utilizing hydrogen, whereas it diminishes by only 12% in ammonia systems. This disparity is attributed to the battery supplying a greater proportion of energy to the powertrain in ammonia systems, thereby reducing the energy demand on the SOFC. Given the efficiency and power characteristics of SOFCs, a lesser efficiency decline is expected in NH3-SOFC systems. This indicates that NH3-SOFC systems potentially offer better fuel consumption efficiency, particularly in EoL scenarios.

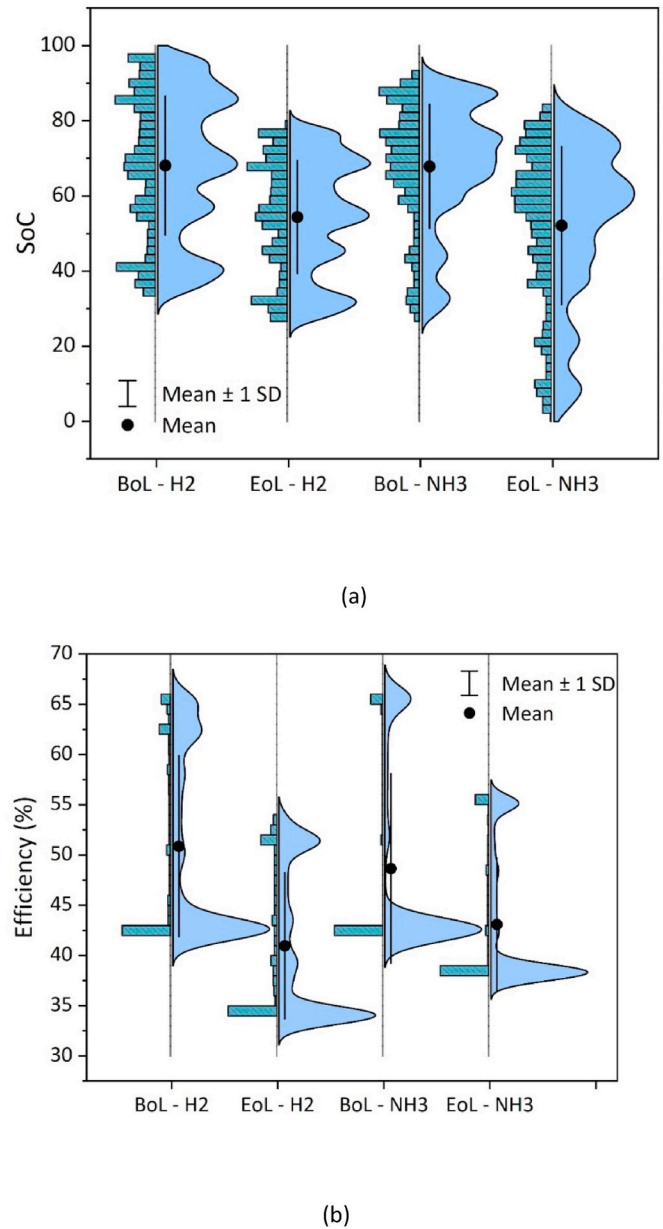


Fig. 8. Performance at Bol and Eol of SOFC and battery: a) state of charge; b) efficiency of SOFC.

5.2. Optimization solution

In this section, simulations are conducted to assess the performance of the proposed SOFC train using two different fuels: hydrogen and ammonia, as detailed in Section 2. The design approach is constrained by space limitations with the objective of minimizing LCOE. Based on the sensitive analysis results of SoC in section 5.1.1, although the 30–70% range is the most economically efficient for both cases, there is a higher possibility of extreme values occurring in ammonia case below 20%, which is detrimental to battery lifetime. To avoid the impact of extreme situations, 20%–85% range has been applied for comparison. For both systems, the minimum and maximum SoC limits are set at 0.2 and 0.85, respectively, with an initial SoC value of 0.8 at the beginning of the driving cycle.

The results of the component sizing optimization problem are presented in Table 5. The findings indicate that the NH3 case requires more battery capacity and space, but it offers better economic efficiency and reduces computational complexity compared to the H2 case. The NH3-

Table 5

Results of SOFC trains powered by hydrogen and ammonia at BoL and EoL.

Design scenario		SOFC size	Battery size	Fuel	LCOE	Time	Engine room
		x 300 kW	x 100 kWh	kg/100 km	£/kWh	s	%
H2-SOFC	BoL	8	20	168	0.406	174.657	+1.5%
	EoL	10	25	197	0.474	130.3383	+24%
NH3-SOFC	BoL	6	24	988	0.267	113.151	+119%
	EoL	8	20	1016	0.332	56.73	+127%

SOFC system reaches the optimal solution in a shorter simulation time, approximately 40% less than the H2-SOFC. This is due to the variable operating temperature of the H2-SOFC, resulting in more computational steps and time required to evaluate power requirements and decide whether to activate the fuel for heating or cooling the SOFC. Additionally, the NH3-SOFC offers cost savings of approximately £0.139/kWh compared to the H2-SOFC at BoL, as shown in Table 5. This is around 30% less, due to the lower cost of fuel and tanks, despite the increased battery size.

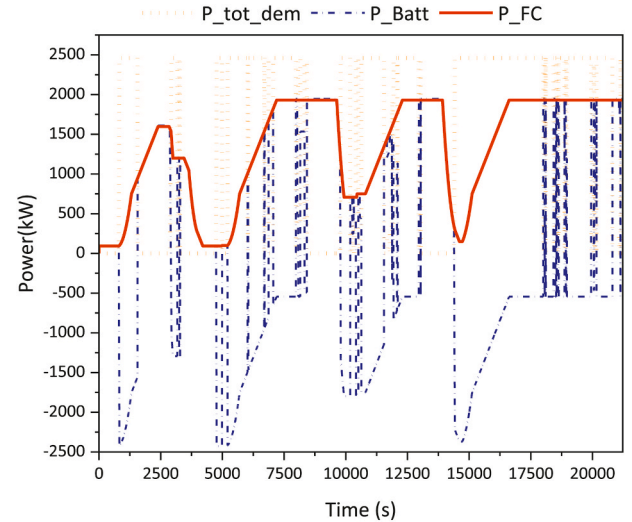
However, due to the additional ammonia crackers and the increased need for batteries in the NH3-SOFC train, an extra wagon is required for this configuration. In this setup, the cracker and fuel tanks can be accommodated in a single wagon, while the hydrogen produced after ammonia decomposition is transported across two carriages. Siemens Mobility has applied for a patent (DE102019203105A1) to facilitate the transfer of hydrogen across cars using a mechanically flexible transport hose [85].

Fig. 9 illustrates the power distribution between the two cases, as well as the power requests for both cases. It is evident that the battery output exhibits a more variable power profile, while the SOFC supplies a more constant power source. This difference is particularly pronounced after 17,500 s in the H2-SOFC case and after 7500 s in the NH3-SOFC case. The higher frequency of power requirement changes results in a more constant power output from the SOFC. However, due to the slow and gradual heat-up process of the SOFC, it cannot immediately adjust its power output like the battery. Consequently, the lower transient capabilities of the SOFC place higher demands on the battery's transient response.

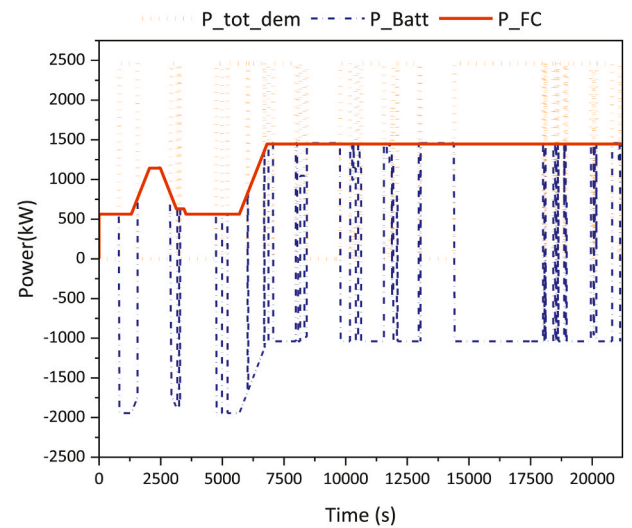
The maximum output power of the battery in the H2-SOFC case is significantly higher than that in the NH3-SOFC case, even though NH3-SOFC has more battery capacity. The maximum battery output occurs at startup when the SOFC cannot provide sufficient power immediately. The SOFC stacks reduce their power output when there is a sustained lower power demand, such as during stops and when the battery's SoC remains within the desired range of 20%–85%. In contrast, the battery's power output in the H2-SOFC case is lower when the SOFC can provide a consistent power source. This is due to the application of more SOFC stacks in H2-SOFC.

In the case of NH3-SOFC, the performance of the SOFC is considerably more stable than in H2-SOFC, especially during the latter half of the drive cycle. To ensure the ammonia cracker operates at the optimal conditions and achieve 100% ammonia decomposition at 1073 K, SOFCs are controlled to operate under a certain temperature, thereby, minimizing disturbance to ammonia cracker. This results in stable power output and less fluctuations in the NH3-SOFC system. However, in the H2-SOFC system, to reduce the heat energy demand and increase powertrain efficiency, the system is designed to allow lower temperature and lower power output, as discussed in Section 4.3 on EMS. This control strategy of the H2-SOFC system introduces more fluctuations and spikes in the power profiles.

After 7500 s, the SOFC operates at an average power output of 1490 kW, while the battery provides approximately 1050 kW. The SOFC dominates the powertrain during stops, startups, acceleration, and deceleration, contributing around 58.6% of the primary power. The additional batteries also contribute to a more stable power supply and maintain less variability in SoC, which can extend battery life.



(a)



(b)

Fig. 9. SOFC and battery power profiles as imposed by the power management in the case of hydrogen-SOFC(a) and ammonia-SOFC (b) train.

The simulation results of the battery SoC are presented in Fig. 10. Different battery operating conditions, determined by the implemented EMS, result in varying SoC profiles. The minimum and maximum SoC values were set at 20% and 80%, respectively. However, both SoC profiles exceed this range, particularly in the case of NH3-SOFC, where the SoC reaches up to 95%. This behavior is due to the SoC being controlled by penalties. When the SoC exceeds the set range, additional costs are incurred. This relaxed control allows the SoC to exceed 85%

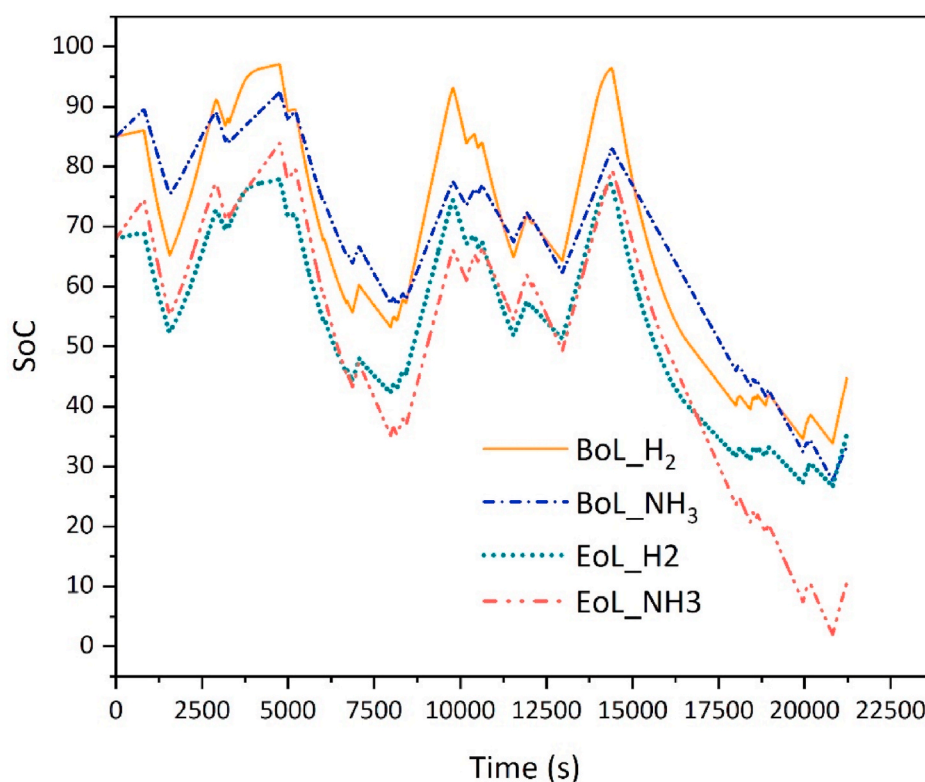


Fig. 10. Battery state of charge profile.

without compromising the power supply. Nevertheless, the minimum SoC for both cases remains above 20%. For Li-ion batteries, overcharging and over-discharging can reduce their lifespan. NH₃-SOFC has several advantages over batteries, including performance and economic benefits.

Both cases exhibit a similar trend, but H₂-SOFC has higher SoC peaks (exceeding 85%) compared to NH₃-SOFC due to greater power demand from the battery during startup. The SoC of NH₃-SOFC remains within the desired range for approximately 95% of the time due to the increased battery capacity and stable power requirements. The simulation results also demonstrate that the SOFC can charge the battery to an 80% SoC during stop times (2500–5000s, 7500–10000s, and 12,500–15000s). Conversely, the battery must supply more power during phases with variable power demands. For instance, after 17500s, the battery's performance varies with changing power requirements. The SoC in both cases gradually decreases until the final stop. This indicates that drive-cycles with more stops provide advantages for the performance of the SOFC powertrain. Energy recovery during deceleration and stops might further enhance battery performance in response to variable power demands.

The fuel consumption is illustrated in Fig. 11. H₂-SOFC requires 58,000 MJ of hydrogen, while NH₃-SOFC necessitates 130,000 MJ (including the combustion fuel for heating) at BoL. Similar to the SoC simulation, the hydrogen-based SOFC exhibits a higher fuel consumption rate due to the increased power demand (Fig. 11 (a)). It's evident that NH₃-SOFC trains produce fewer power peaks compared to SOFCs fueled by hydrogen (Fig. 9). H₂-SOFC exhibits higher average efficiency than NH₃-SOFC due to the more frequent peaks during the latter half of the drive cycle (Fig. 12). However, in both cases, the SOFCs operate at a constant power efficiency of 42% at BoL. According to Eq. (9), when SOFC stacks produce higher power output, the fuel cell's efficiency decreases. This is clearly observed during the startup of the SOFC, where low power output corresponds to very high efficiency.

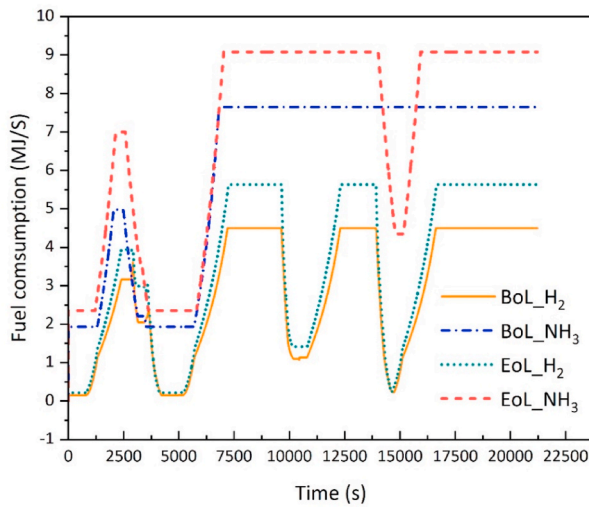
The efficiency trends align with the variation in mass flow rates entering the SOFC anode (Eq. (9)), which are influenced by the active

species. The simulation results from Figs. 11 and 12 indicate that lower mass flow rates lead to higher efficiency. Efficiency and mass flow rates are also linked to the operating temperature, which in turn affects the current and voltage performance.

Fig. 13 displays the temperature profiles of the SOFC stacks. NH₃-SOFC maintains a temperature of 1073 K because the inlet fuel originates from the ammonia cracker, which matches the SOFC's operating temperature. In H₂-SOFC, the temperature varies between 875 K and 1073 K to meet power demand requirements. H₂-SOFC's efficiency is more complex than NH₃-SOFC due to the two variables: mass flow rate and temperature. On the other hand, NH₃-SOFC's power output changes solely due to variations in mass flow rate. This is evident around 10,000s and 15,000s, where temperatures are approximately 950 K and 873 K, respectively. However, their efficiencies tend to become similar. In line with Fig. 12, higher operating temperatures require more fuel for heating the SOFC module.

To illustrate the spatial feasibility of the design, a 3D CAD model of hydrogen-fueled SOFC train has been created using data obtained from the Class 66's dimensions. The design is presented in Fig. 14. As is common with most storage systems in demonstrator, prototype, and ordered railway vehicles, these systems are typically mounted on the roof or inside the machine house. In this study, hydrogen tanks are positioned near the roof due to the fact that, in case of a failure, hydrogen tends to dissipate upwards when stored under pressure. However, they are also situated within the machine house due to the height restrictions of British rail tunnels.

In the case of the H₂-SOFC train, the carriage is filled with tanks, SOFC units, and batteries. Notably, certain batteries are arranged beneath the locomotive to replace the original diesel tanks. Modeling has shown that the selected fuel cells and batteries not only meet the power demands but also fit within the volume of one Class 66 locomotive without affecting cargo capacity. Conversely, the NH₃-SOFC system is more expensive compared to the hydrogen-SOFC, albeit with a compromise on capacity. The NH₃-SOFC train, similar in structure to its hydrogen counterpart but with an additional wagon for ammonia tanks,



(a)

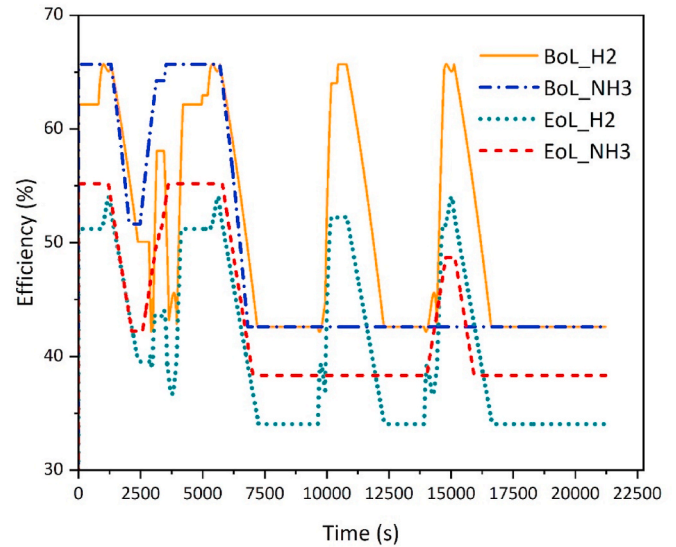
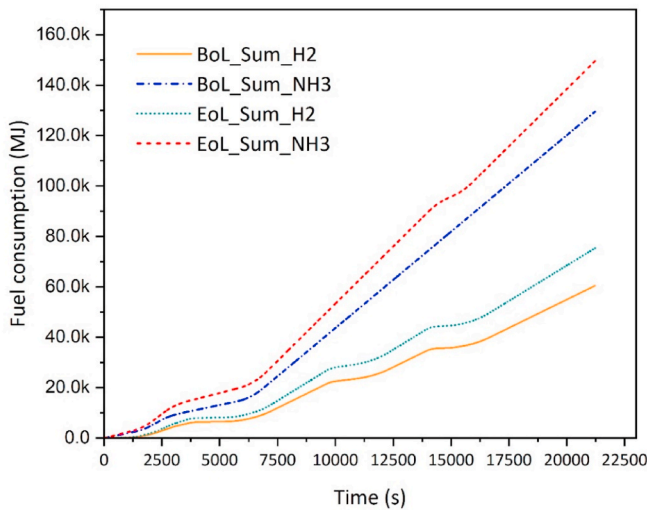


Fig. 12. Efficiency of SOFC in two scenarios.



(b)

Fig. 11. a) Fuel consumption rate; b) fuel consumption.

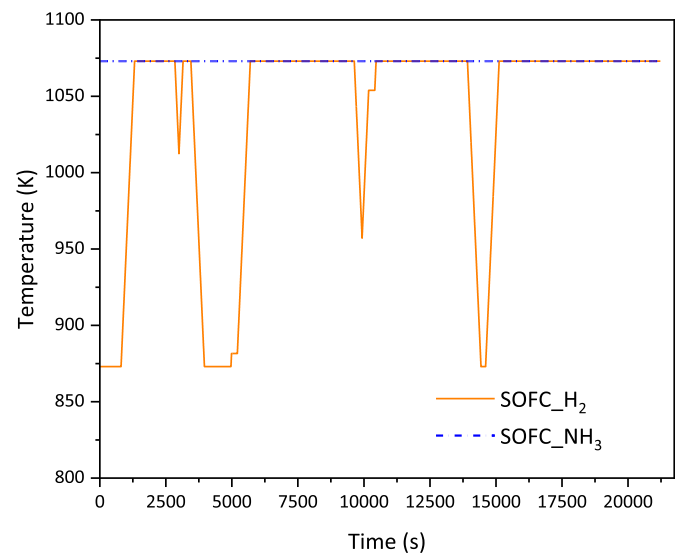


Fig. 13. Operating temperature of SOFC.

would not have its detailed 3D model showcased here.

6. Conclusion

This paper introduces the design of an MW-scale hybrid freight train using either hydrogen or ammonia-fueled SOFCs, offering a strategic pathway towards decarbonized traction. Findings suggest that ammonia-fueled SOFC trains could potentially reduce LCOE by 30% compared to their hydrogen counterparts, owing to inexpensive ammonia fuel cost. It is interesting to note that high pressure compressive hydrogen storage requires less additional space in engine compartments, mainly due to the external ammonia cracker using extra space.

In this study, PSO is utilized to determine the sizing of the main power sources, including SOFCs and batteries, while applying the total wagon space usage as a constraint and the LCOE as the objective function. The parametric analysis examines key variables such as SoC, startup duration, end-of-life efficiency of the proposed systems and the PSO weighting and penalty are analyzed to reveal their implications on

the optimization algorithm. This provides insights into the optimal sizing ratio for SOFCs and batteries in the powertrain system of freight trains.

Regarding the operational range of SoC, no specific standard in transportation applications has been implemented. The SoC of batteries in the hybrid SOFC freight train is recommended to be maintained within the range of 50–80%, which has a relatively higher overall economy. Although the case with SoC in the range of 30%–70% shows even better economy in terms of LCOE, the powertrain system demonstrates larger fluctuations, which may lead to increasing degradation of the batteries. It is also approved in other literature that the SoC range of 50–80% resulted in a moderate decrease of 1% for the inner resistance and less than 5% capacity degradation of the batteries.

The hybrid ammonia-fueled SOFC freight train shows economic advantages throughout the lifespan (both BoL and EoL). If the hybrid powertrain is designed based on the worst-case scenario using EoL performance profiles of SOFCs and batteries, both hydrogen and ammonia cases required additional 600 kW SOFC stacks than the design scenario using BoL performance profiles. Due to the temperature maintenance requirement of the ammonia cracker in the ammonia case,

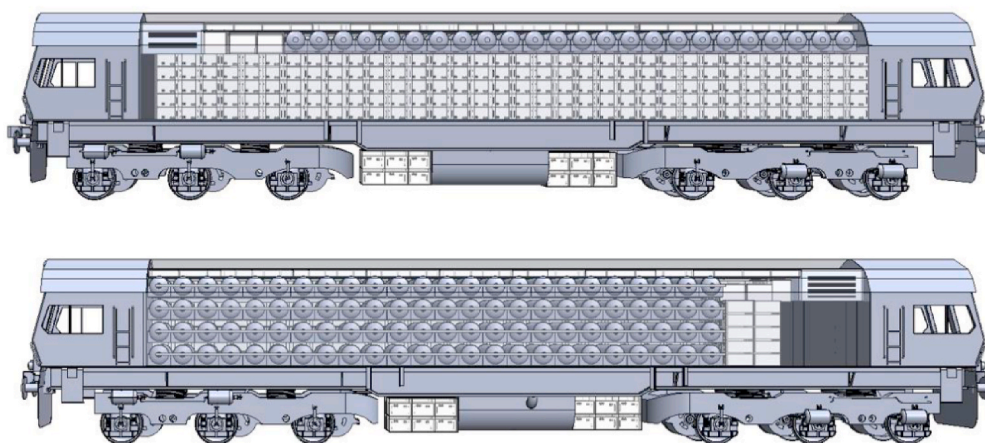


Fig. 14. 3D model of Hydrogen SOFC train.

the cracker assists to stabilize the feed-in fuel temperature of SOFCs, in turn, fewer thermal cycles and less degradation of ammonia fueled SOFCs. The power profile of ammonia fueled SOFCs evidences its stable operation with 60% time working on a constant load. With less degradation of ammonia fueled SOFCs, the fuel consumption for the ammonia case increased by only 2.8%, whereas for hydrogen, it surged by 17.3%, therefore the ammonia-fueled SOFC outperformed the hydrogen case by 5% in efficiency at EoL. This also results in the hydrogen case being 0.142 £/kWh more costly.

Overall, this study suggests that employing SOFCs in the subsector of freight train is feasible. The adaptability of SOFCs to various fuels leads to different design solutions using either hydrogen or ammonia as a main fuel of freight trains. Both solutions of zero carbon fuels achieve decarbonized traction, with the goal of replacing diesel-powered passenger rolling stock by 2040. However, while the ammonia option offers the economic advantage and improved SOFC performance at EoL, it requires one extra wagon to accommodate more ammonia storage tanks (the ammonia cracker takes space in the locomotive), a significant trade-off for asset owners and operators. Further enhancements for ammonia fueled hybrid powertrain solutions may aim at compactness (power density of SOFCs and energy density of ammonia storage), system integration (integrating of cracker and SOFCs) and additional cost reduction (both SOFCs and batteries) better suited for freight trains and other heavy transport applications.

CRediT authorship contribution statement

Yuqi Zhang: Conceptualization, Investigation, Methodology, Writing – original draft, Writing – review & editing. **Jiacheng Yu:** Data curation, Formal analysis, Investigation, Writing – original draft. **Ning Zhao:** Conceptualization, Methodology, Validation. **Zhan Xu:** Conceptualization, Methodology. **Yan Yan:** Methodology, Validation. **Dawei Wu:** Conceptualization, Funding acquisition, Resources, Supervision, Writing – original draft, Writing – review & editing. **Kevin Blacktop:** Resources. **Athanasios Tsolakis:** Funding acquisition, Resources.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Dawei Wu reports financial support was provided by Engineering and Physical Sciences Research Council. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The authors are grateful for the financial support from EPSRC (Engineering and Physical Sciences Research Council, United Kingdom) through the projects EP/S00193X/2 and EP/W016656/1.

References

- [1] Committee TMCC, Stark C. Net Zero the UK's contribution to stopping global warming. Committee on Climate Change. 2019. p. 142 [Online]. Available: www.theccc.org.uk/publications.
- [2] James BD, Houchins C, Huya-Kouadio JM, Desantis DA. Final report: hydrogen storage system cost analysis 2016. 2016 [Online]. Available: www.sainc.com.
- [3] Benmouna A, Becherif M, Boulon L, Dépature C, Ramadan HS. Efficient experimental energy management operating for FC/battery/SC vehicles via hybrid Artificial Neural Networks-Passivity Based Control. *Renew Energy* Nov. 2021;178: 1291–302. <https://doi.org/10.1016/j.renene.2021.06.038>.
- [4] Calvert C, Allan J, Amor P, Hillmans S, Roberts C, Weston P. Concept development and testing of the UK's first hydrogen-hybrid train (HydroFLEX). *Railway Engineering Science* Sep. 2021;29(3):248–57. <https://doi.org/10.1007/s40534-021-00256-9>.
- [5] Haseltalab A, van Biert L, Sapra H, Mestemaker B, Negenborn RR. Component sizing and energy management for SOFC-based ship power systems. *Energy Convers Manag* Oct. 2021;245. <https://doi.org/10.1016/j.enconman.2021.114625>.
- [6] Palmer C. Hydrogen-powered trains start to roll. *Engineering* Apr. 2022;11:9–11. <https://doi.org/10.1016/j.eng.2022.02.003>.
- [7] Hoffrichter A, Hillmans S, Roberts C. Conceptual propulsion system design for a hydrogen-powered regional train. *IET Electr Syst Transp* Jun. 2016;6(2):56–66. <https://doi.org/10.1049/iet-est.2014.0049>.
- [8] Xu Z, Zhao N, Hillmans S, Roberts C, Yan Y. Techno-economic analysis of hydrogen storage technologies for railway engineering: a review. *Energies* Sep. 01, 2022;15(17). <https://doi.org/10.3390/en15176467>.
- [9] Lee S, et al. Reliable sealing design of metal-based solid oxide fuel cell stacks for transportation applications. *Int J Hydrogen Energy* Nov. 2019;44(57):30280–92. <https://doi.org/10.1016/j.ijhydene.2019.09.087>.
- [10] Gong C, Xu Y, Cai S, Chi B, Tu Z. Comparative study on thermodynamic analysis of solid oxide fuel cells supplied with methanol or ammonia. *Int J Hydrogen Energy* Jan. 2024;50:1293–301. <https://doi.org/10.1016/j.ijhydene.2023.10.266>.
- [11] Mendez C, Contestabile M, Bicer Y. Hydrogen fuel cell vehicles as a sustainable transportation solution in Qatar and the Gulf cooperation council: a review. *Int J Hydrogen Energy* Dec. 2023;48(99):38953–75. <https://doi.org/10.1016/j.ijhydene.2023.04.194>.
- [12] Yan H, et al. Techno-economic evaluation and technology roadmap of the MWe-scale SOFC-PEMFC hybrid fuel cell system for clean power generation. *J Clean Prod* May 2020;255:120225. <https://doi.org/10.1016/j.jclepro.2020.120225>.
- [13] Al-Hamed KHM, Dincer I. A novel ammonia solid oxide fuel cell-based powering system with on-board hydrogen production for clean locomotives. *Energy* 2021; 220(Apr). <https://doi.org/10.1016/j.energy.2021.119771>.
- [14] Rechberger J, Kaupert A, Hagerskans J, Blum L. Demonstration of the first European SOFC APU on a heavy duty truck. *Transport Res Procedia* Jan. 2016;14: 3676–85. <https://doi.org/10.1016/j.trpro.2016.05.442>.
- [15] Kendall K. SOFC APU for auxiliary road-truck installations. 2017 [Online]. Available: . [Accessed 12 October 2023].
- [16] Andersson M, Sundén B. Technology review-solid oxide fuel cell [Online]. Available: www.energiforsk.se; 2017.
- [17] Ling-Chin J, et al. Technology roadmap for hydrogen-fuelled transportation in the UK. *Int J Hydrogen Energy* Jan. 2024;52:705–33. <https://doi.org/10.1016/j.ijhydene.2023.04.131>.

- [18] Mylonopoulos F, Polinder H, Coraddu A. A comprehensive review of modeling and optimization methods for ship energy systems. *IEEE Access* 2023;11:32697–707. <https://doi.org/10.1109/ACCESS.2023.3263719>.
- [19] IEEE Power & Energy Society, IEEE Power Electronics Society, IEEE international conference on service-oriented computing and applications, va. IEEE electric ship technologies symposium 6 2015.06.21–24 alexandria, va. Biennial electric ship technologies symposium 6 2015.06.21–24 alexandria, and va. ESTS 6 2015.06.21–24 alexandria, 2015 IEEE electric ship technologies symposium (ESTS) 21–24 june 2015, alexandria, VA..
- [20] Valera-Garcia JJ, Atutxa-Lekue I. On the optimal design of hybrid-electric power systems for offshore vessels. *IEEE Transactions on Transportation Electrification* Mar. 2019;5(1):324–34. <https://doi.org/10.1109/TTE.2018.2883870>.
- [21] Lan H, Wen S, Hong YY, Yu DC, Zhang L. Optimal sizing of hybrid PV/diesel/battery in ship power system. *Appl Energy* Nov. 2015;158:26–34. <https://doi.org/10.1016/J.APENERGY.2015.08.031>.
- [22] Hein K, Xu Y, Wilson G, Gupta AK. Coordinated optimal voyage planning and energy management of all-electric ship with hybrid energy storage system. *IEEE Trans Power Syst* May 2021;36(3):2355–65. <https://doi.org/10.1109/TPWRS.2020.3029331>.
- [23] Dolatabadi A, Mohammadi-Ivatloo B. Stochastic risk-constrained optimal sizing for hybrid power system of merchant marine vessels. *IEEE Trans Ind Inf Dec.* 2018;14(12):5509–17. <https://doi.org/10.1109/TII.2018.2824811>.
- [24] Kanellos FD. Optimal power management with GHG emissions limitation in all-electric ship power systems comprising energy storage systems. *IEEE Trans Power Syst* Jan. 2014;29(1):330–9. <https://doi.org/10.1109/TPWRS.2013.2280064>.
- [25] Kanellos FD, Anvari-Moghaddam A, Guerrero JM. A cost-effective and emission-aware power management system for ships with integrated full electric propulsion. *Elect Power Syst Res* Sep. 2017;150:63–75. <https://doi.org/10.1016/J.EPSR.2017.05.003>.
- [26] Wu P, Bucknall R. Hybrid fuel cell and battery propulsion system modelling and multi-objective optimisation for a coastal ferry. *Int J Hydrogen Energy* Jan. 2020;45(4):3193–208. <https://doi.org/10.1016/J.IJHYDENE.2019.11.152>.
- [27] Dall'Armi C, Pivetta D, Taccani R. Uncertainty analysis of the optimal health-conscious operation of a hybrid PEMFC coastal ferry. *Int J Hydrogen Energy* Mar. 2022;47(21):11428–40. <https://doi.org/10.1016/J.IJHYDENE.2021.10.271>.
- [28] Soleymani M, Yoozofi A, Kandi-D M. Sizing and energy management of a medium hybrid electric boat. *J Mar Sci Technol Dec.* 2015;20(4):739–51. <https://doi.org/10.1007/s00773-015-0327-0>.
- [29] Mohamad Izdin Hlal A, Ramachandaramurthy VK, Sanjeevikumar Padmanaban B, Hamid Reza Kaboli C, Aref Pouryekt A, Tuan Ab Rashid Bin Tuan Abdullah D. NSGA-II and MOPSO based optimization for sizing of hybrid PV/wind/battery energy storage system. *Int J Power Electron Drive Syst* Mar. 2019;10(1):463–78. <https://doi.org/10.11591/ijpeds.v10.i1.pp463-478>.
- [30] Zhu J, Chen L, Wang B, Xia L. Optimal design of a hybrid electric propulsive system for an anchor handling tug supply vessel. *Appl Energy* Sep. 2018;226:423–36. <https://doi.org/10.1016/J.APENERGY.2018.05.131>.
- [31] Heleno M, Mashayekh S, Stadler M, Cardoso G, De Luís R. Optimal sizing and placement of distributed generation: MILP vs PSO comparison in a real microgrid application. 2017.
- [32] Chourasia V, Pandey S, Kumar S. Optimizing the performance of vehicular delay tolerant networks using multi-objective PSO and artificial intelligence. *Comput Commun Sep.* 2021;177:10–23. <https://doi.org/10.1016/J.COMCOM.2021.06.006>.
- [33] Wang X, Shipurkar U, Haseltalab A, Polinder H, Claeys F, Negenborn RR. Sizing and control of a hybrid ship propulsion system using multi-objective double-layer optimization. *IEEE Access* 2021;9:72587–601. <https://doi.org/10.1109/ACCESS.2021.3080195>.
- [34] Zhang C, et al. Dedicated adaptive particle swarm optimization algorithm for digital twin based control optimization of the plug-in hybrid vehicle. *IEEE Transactions on Transportation Electrification* Jun. 2023;9(2):3137–48. <https://doi.org/10.1109/TTE.2022.3219290>.
- [35] Zhang C, Zhou Q, Li Y, Hua L, Xu H. The digital twin modelling of the electrified vehicle based on A hybrid terminating control of particle swarm optimization. *IFAC-PapersOnLine* Jan. 2021;54(10):552–7. <https://doi.org/10.1016/J.IFACOL.2021.10.220>.
- [36] Sarma U, Ganguly S. Design optimisation for component sizing using multi-objective particle swarm optimisation and control of PEM fuel cell/battery hybrid energy system for locomotive application. *IET Electr Syst Transp* Mar. 2020;10(1):52–61. <https://doi.org/10.1049/iet-est.2018.5053>.
- [37] Sarma U, Ganguly S. Determination of the component sizing for the PEM fuel cell-battery hybrid energy system for locomotive application using particle swarm optimization. *J Energy Storage* Oct. 2018;19:247–59. <https://doi.org/10.1016/J.EST.2018.08.008>.
- [38] Zhang Y, Tian Z, Roberts C, Hillmans S, Chen M. Cost optimization of multi-mode train conversion for discontinuously electrified routes. *Int J Electr Power Energy Syst* 2022;138(Jun). <https://doi.org/10.1016/j.ijepes.2022.107993>.
- [39] Zhu J, Chen L, Wang X, Yu L. Bi-level optimal sizing and energy management of hybrid electric propulsion systems. *Appl Energy* Feb. 2020;260:114134. <https://doi.org/10.1016/J.APENERGY.2019.114134>.
- [40] Barelli L, Bidini G, Ciupăgeanu DA, Pianese C, Polverino P, Sorrentino M. Stochastic power management approach for a hybrid solid oxide fuel cell/battery auxiliary power unit for heavy duty vehicle applications. *Energy Convers Manag* Oct. 2020;221:113197. <https://doi.org/10.1016/J.ENCONMAN.2020.113197>.
- [41] Besekon Y, Zielke P, Wulff AC, Hagen A. Simulation of a SOFC/Battery powered vehicle. *Int J Hydrogen Energy* Jan. 2019;44(3):1905–18. <https://doi.org/10.1016/J.IJHYDENE.2018.11.126>.
- [42] Wu Xu Y, et al. Development of solid oxide fuel cell and battery hybrid power generation system. *Int J Hydrogen Energy* Mar. 2020;45(15):8899–914. <https://doi.org/10.1016/J.IJHYDENE.2020.01.032>.
- [43] Rathore SS, Biswas S, Fini D, Kulkarni AP, Giddey S. Direct ammonia solid-oxide fuel cells: a review of progress and prospects. *Int J Hydrogen Energy* Oct. 2021;46(71):35365–84. <https://doi.org/10.1016/J.IJHYDENE.2021.08.092>.
- [44] Wu S, Miao B, Chan SH. Feasibility assessment of a container ship applying ammonia cracker-integrated solid oxide fuel cell technology. *Int J Hydrogen Energy* Jul. 2022;47(63):27166–76. <https://doi.org/10.1016/J.IJHYDENE.2022.06.068>.
- [45] Office of Rail and Road, “Freight rail usage and performance July to September 2023.”.
- [46] van Biert L, Godjevac M, Visser K, Aravind PV. A review of fuel cell systems for maritime applications. *J Power Sources* Sep. 2016;327:345–64. <https://doi.org/10.1016/J.JPOWSOUR.2016.07.007>.
- [47] Xiong G, Zhang J, Shi D, Yuan X. A simplified competitive swarm optimizer for parameter identification of solid oxide fuel cells. *Energy Convers Manag* Jan. 2020;203:112204. <https://doi.org/10.1016/J.ENCONMAN.2019.112204>.
- [48] Safari S, Hajilounzad T, Ehyaei MA. Multi-objective optimization of solid oxide fuel cell/gas turbine combined heat and power system: a comparison between particle swarm and genetic algorithms. *Int J Energy Res* Sep. 2020;44(11):9001–20. <https://doi.org/10.1002/er.5610>.
- [49] Hoffrichter A, Fisher P, Tutchter J, Hillmans S, Roberts C. Performance evaluation of the hydrogen-powered prototype locomotive ‘Hydrogen Pioneer’. *J Power Sources* Mar. 2014;250:120–7. <https://doi.org/10.1016/j.jpowsour.2013.10.134>.
- [50] Din T, Hillmans S. Energy consumption and carbon dioxide emissions analysis for a concept design of a hydrogen hybrid railway vehicle. *IET Electr Syst Transp* Jun. 2018;8(2):112–21. <https://doi.org/10.1049/iet-est.2017.0049>.
- [51] Zhang Y, et al. A techno-economic analysis of ammonia-fuelled powertrain systems for rail freight. *Transp Res D Transp Environ* Jun. 2023;119:103739. <https://doi.org/10.1016/J.TRD.2023.103739>.
- [52] GB Railway Data Ltd, “Route Viewer - RailMaps.”.
- [53] Barelli L, Bidini G, Ciupăgeanu DA, Pianese C, Polverino P, Sorrentino M. Stochastic power management approach for a hybrid solid oxide fuel cell/battery auxiliary power unit for heavy duty vehicle applications. *Energy Convers Manag* Oct. 2020;221:113197. <https://doi.org/10.1016/J.ENCONMAN.2020.113197>.
- [54] van Veldhuizen BN, van Biert L, Amladi A, Woudstra T, Visser K, Aravind PV. The effects of fuel type and cathode off-gas recirculation on combined heat and power generation of marine SOFC systems. *Energy Convers Manag* Jan. 2023;276:116498. <https://doi.org/10.1016/J.ENCONMAN.2022.116498>.
- [55] Kishimoto M, et al. Development of 1 kW-class ammonia-fueled solid oxide fuel cell stack. *Fuel Cell* Feb. 2020;20(1):80–8. <https://doi.org/10.1002/fuce.201900131>.
- [56] Cesaro Z, Ives M, Nayak-Luke R, Mason M, Bañares-Alcántara R. Ammonia to power: forecasting the leveled cost of electricity from green ammonia in large-scale power plants. *Appl Energy* Jan. 2021;282. <https://doi.org/10.1016/j.apenergy.2020.116009>.
- [57] Ku B-Y, September 2021 Land Transportation News [Transportation Systems]. *IEEE Veh Technol Mag* Aug. 2021;16(3):14–7. <https://doi.org/10.1109/mvt.2021.3089845>.
- [58] USDoe. DOE technical targets for onboard hydrogen storage for light-duty vehicles _ department of energy [Online]. Available: <https://www.energy.gov/eere/fuelcells/doe-technical-targets-onboard-hydrogen-storage-light-duty-vehicles>. [Accessed 1 March 2024].
- [59] Elcogen, “Solid oxide stacks for fuel cell systems – Affordable Green Hydrogen.” Accessed: Jan. 24, 2024. [Online]. Available: <https://elcogen.com/products/solid-oxide-stacks-for-fuel-cell-systems/>.
- [60] H. P. A. M., Ammermann H, et al. Advancing Europe’s energy systems-stationary fuel cells in distributed generation. 2015 [J].
- [61] OSN Power, “OSN Power Energy Limited-sfhy.com.” Accessed: Jan. 24, 2024. [Online]. Available: <https://www.eurotainer.com/containers/>.
- [62] E. & I. S. Department for Business. Hydrogen production costs 2021. 2021.
- [63] Luxfer, “Hydrogen - Luxfer Gas Cylinders.” Accessed: Jan. 24, 2024. [Online]. Available: <https://www.luxfercylinders.com/application/hydrogen/#:~:text=Luxfer%27s%20G%2Dstor%C2%AE%20Pro,cells%20and%20internal%2Dcombustion%20engines..>
- [64] Jackson C, et al. Ammonia to green hydrogen project feasibility study. 2019.
- [65] Eurotainer, “Containers - Eurotainer.” Accessed: Jan. 24, 2024. [Online]. Available: <https://www.eurotainer.com/containers/>.
- [66] Elishav O, Mosevitzky Lis B, Valera-Medina A, Grader GS. Storage and distribution of ammonia. Techno-economic challenges of green ammonia as an energy vector. *Jan. 2021. p. 85–103. https://doi.org/10.1016/B978-0-12-820560-0.00005-9*.
- [67] Fúnez Guerra C, Reyes-Bozo L, Vyhmeister E, Jaén Caparrós M, Salazar JL, Clemente-Jul C. Technical-economic analysis for a green ammonia production plant in Chile and its subsequent transport to Japan. *Renew Energy* Sep. 2020;157:404–14. <https://doi.org/10.1016/j.renene.2020.05.041>.
- [68] Royal Society. Ammonia: zero-carbon fertiliser, fuel and energy store [J]. 2021.
- [69] Wu Z, et al. Dynamic modeling and operation strategy of an NG-fueled SOFC-WGS-TSA-PEMFC hybrid energy conversion system for fuel cell vehicle by using MATLAB/SIMULINK. *Energy* May 2019;175:567–79. <https://doi.org/10.1016/J.ENERGY.2019.03.119>.
- [70] Zhao F, Virkar AV. Dependence of polarization in anode-supported solid oxide fuel cells on various cell parameters. *J Power Sources* Feb. 2005;141(1):79–95. <https://doi.org/10.1016/J.JPOWSOUR.2004.08.057>.

- [71] Zaghib K, et al. Safe and fast-charging Li-ion battery with long shelf life for power applications. *J Power Sources* Apr. 2011;196(8):3949–54. <https://doi.org/10.1016/j.jpowsour.2010.11.093>.
- [72] Soper D, Baker C, Sterling M. Experimental investigation of the slipstream development around a container freight train using a moving model facility. *J Wind Eng Ind Aerod Dec*. 2014;135:105–17. <https://doi.org/10.1016/j.jweia.2014.10.001>.
- [73] Lin Y, Xin D, Bian X, Zhang Q, Li T. Improved adaptive inertia weight PSO algorithm and its application in nuclear power pipeline layout optimization. *Chinese Journal of Ship Research* 2023;18(3). <https://doi.org/10.19693/j.issn.1673-3185.02940>.
- [74] Cec 2003 : the 2003 congress on evolutionary computation : [proceedings] : canberra, Australia, 8-12 december, 2003. IEEE; 2003.
- [75] National Renewable Energy Laboratory (NREL), “Utility-Scale Battery Storage.” Accessed: May 27, 2022. [Online]. Available: <https://atb.nrel.gov/electricity/2021/utility-scale-battery-storage>.
- [76] Apostolou D. Refuelling scenarios of a light urban fuel cell vehicle with metal hydride hydrogen storage. Comparison with compressed hydrogen storage counterpart. *Int J Hydrogen Energy* Nov. 2021;46(79):39509–22. <https://doi.org/10.1016/j.ijhydene.2021.09.157>.
- [77] Nayak-Luke RM, Forbes C, Cesaro Z, Bañares-Alcántara R, Rouwenhorst KHR. Techno-economic aspects of production, storage and distribution of ammonia. In: Techno-economic challenges of green ammonia as an energy vector. Elsevier; 2021. p. 191–207. <https://doi.org/10.1016/b978-0-12-820560-0.00008-4>.
- [78] Minutillo M, Perma A, Di Trollo P, Di Micco S, Jannelli E. Techno-economics of novel refueling stations based on ammonia-to-hydrogen route and SOFC technology. *Int J Hydrogen Energy* Mar. 2021;46(16):10059–71. <https://doi.org/10.1016/j.ijhydene.2020.03.113>.
- [79] Chahbaz A, Meishner F, Li W, Ünlibayir C, Uwe Sauer D. Non-invasive identification of calendar and cyclic ageing mechanisms for lithium-titanate-oxide batteries. *Energy Storage Mater* Nov. 2021;42:794–805. <https://doi.org/10.1016/j.ensm.2021.08.025>.
- [80] Dokiya M. SOFC system and technology. *Solid State Ionics* Dec. 2002;152–153: 383–92. [https://doi.org/10.1016/S0167-2738\(02\)00345-4](https://doi.org/10.1016/S0167-2738(02)00345-4).
- [81] long Wu X, et al. Health state prediction and analysis of SOFC system based on the data-driven entire stage experiment. *Appl Energy* Aug. 2019;248:126–40. <https://doi.org/10.1016/j.apenergy.2019.04.053>.
- [82] Hafsia A, Bariza Z, Djamel H, Hocine BM, Andreadis GM, Soumia A. SOFC fuel cell heat production: analysis. *Energy Proc Jan*. 2011;6:643–50. <https://doi.org/10.1016/j.egypro.2011.05.074>.
- [83] Akikur RK, Saidur R, Ping HW, Ullah KR. Performance analysis of a co-generation system using solar energy and SOFC technology. *Energy Convers Manag Mar*. 2014;79:415–30. <https://doi.org/10.1016/j.enconman.2013.12.036>.
- [84] Parhizkar T, Hafeznezami S. Degradation based operational optimization model to improve the productivity of energy systems, case study: solid oxide fuel cell stacks. *Energy Convers Manag Feb*. 2018;158:81–91. <https://doi.org/10.1016/j.enconman.2017.12.045>.
- [85] Böhm M, Fernández Del Rey A, Pagenkopf J, Varela M, Herwartz-Polster S, Nieto Calderón B. Review and comparison of worldwide hydrogen activities in the rail sector with special focus on on-board storage and refueling technologies. *Int J Hydrogen Energy* Nov. 2022;47(89):38003–17. <https://doi.org/10.1016/j.ijhydene.2022.08.279>.

Abbreviations

Auxiliary power unit: APU
BoL: Begin of life
CAPEX: Capital expenditure
DoD: Depth of discharge
EoL: End of life
Energy Management System: EMS
LCOE: Levelized cost of electricity, £/kWh)
LHV: Lower heating value (MJ/kg)
O&M: Maintenance costs
OPEX: Operational Expenditure
Mixed Integer Linear Programming: MILP
Multi-Particle Swarm Optimization: MOPSO
Nitrogen oxides: NO_x
Non-dominated Sorting Genetic Algorithm-II: NSGA-II
Particle Swarm Optimization: PSO
Proton Exchange Membrane Fuel Cells: PEMFCs
Solid Oxide Fuel Cells: SOFCs
State of Charge: SoC

Symbols

a: Anode
act: Activation overvoltage
Batt: Battery
c: Cathode
C: Cost
con: Concentration overvoltage
D: Diffusion coefficient
dem: Power demand
E: Local Nernst potential, V
F: Faraday constant, 96,384 C mol^{−1}
I: Current, A
i: iteration
j: Year in the range of system lifetime
J: Current density, A/m²
K: Equilibrium constant
l: Thickness, m
M: Molar mass, g/mol
m: Mass flow rate, kg/s
n: Anode/cathode
ohm: ohmic overvoltage
P: Pressure, bar
py: Previous year
r: Resistance
rep: Replacement
t: Lifespan of the facility, year
R: Universal gas constant, 8.314 J mol^{−1} K^{−1}
V: Cell voltage, V
η: Overvoltage
η_{cell}: Efficiency of SOFC
ε: Electrode porosity
ζ: Electrode tortuosity