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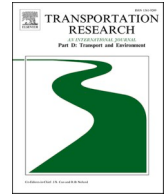
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A techno-economic analysis of ammonia-fuelled powertrain systems for rail freight

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ABSTRACT

All diesel-only trains in the UK will be removed from services by 2040. High volumetric density, rapid refuelling ability, and sophisticated experience in infrastructure and logistics make ammonia a perfect hydrogen carrying fuel for rail freight, which urgently requires an economically viable solution. This study conducted a novel techno-economic study of ammonia-fuelled fuel cell powertrains to be compared with current diesel engine-based system and emerging direct hydrogen-fuelled fuel cell system. The results demonstrate that hydrogen-fuelled Proton-Exchange Membrane Fuel Cells (PEMFCs) and ammonia-fuelled PEMFCs (using an ammonia cracker) are more cost-effective in terms of Levelized Cost of Electricity. The ammonia fuel storage requires 61.5-75 % less space compared to the hydrogen storage. Although the ammonia-fuelled Solid Oxide Fuel Cells (SOFCs) powertrain has the highest electricity generation efficiency (56%), the overall cost requires a major reduction by 70% before it could be considered as an economically viable solution.

1. Introduction

In response to the law of achieving Net Zero Green House Gas emissions in the UK by 2050 (Stark and Committee, 2019), the UK Department for Transport has proposed a target to remove all diesel-only trains off the track by 2040 (James et al., 2016). In recent years, some viable pathways have emerged for achieving this target: electric traction, battery power, and fuel cells, which are at the forefront of environmentally preferable railway traction technologies.

It is widely agreed that electric traction is the optimal choice due to low carbon intensity, light counterparts, and quiet operation compared to diesel traction. The proportion of electrified routes in the UK, as measured by the length of the routes, is approximately 38% with 70% of passenger rail using electric traction in 2020 (Office of Rail and Road, 2021). Research has been performed to improve the electrification energy efficiency based on the fully electrified routes by regenerating energy (Iannuzzi and Tricoli, 2012; Zhang et al., 2019) and optimising train driving strategy (Tian et al., 2017; Wang et al., 2019). However, significant investment and time are required for the electrification of the infrastructure because most tracks in the UK are discontinuously electrified. In 2017, the UK government cancelled the electrification rail projects in the North, the Midlands and Wales due to financial problems (Zhang et al., 2022).

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Nomenclature

Abbreviations

Bol	beginning of life
BP	Battery pack
Cap	capital cost
CAPEX	capital expenditure
CEF	carbon dioxide equivalent factor (g CO _{2e} /MJ)
CO _{2e}	carbon dioxide equivalent emissions (g)
Cracker-PEM	ammonia cracker-PEM drive-system
Cracker-SOFC	ammonia cracker-SOFC drive-system
CVF	calorific value of fuel (J/kg)
DCF	discounted cash flows
DoD	depth of discharge
DPP	discounted Payback Period
EMD-710	diesel-electric drive-system
EoL	end of life
FCS	fuel cell systems
GH2	Compressed gas hydrogen storage technology
H2-PEM	Hydrogen PEMFC drive-system
ICE	internal combustion engine
IEA	International Energy Agency
ISO	International Organization for Standardization
LCOE	levelized cost of electricity (£/kWh)
LHV	lower heating value (MJ/kg)
NAI	Net Annual Income
NH ₃ -SOFC	direct ammonia fuelled SOFC drive-system
O&M	maintenance costs
OPEX	Operational Expenditure
PEMFC	Proton-Exchange Membrane Fuel Cell
REPLEX	Replacement Expenditure
SOFC	Solid Oxide Fuel Cell
TRL	Technology Readiness Level
TTW	tank-to-wheel
WTW	well-to-wheel

Symbols

η	Efficiency
$E_{electricity}$	Annual electricity production
C_{BP}	Cost of battery
C_{BPrep}	Replacement cost of battery
$C_{CRACKER}$	Replacement cost of cracker
$C_{Cracker(NH_3)}$	The percentage conversion of ammonia
C_{FCrep}	Replacement cost of fuel cell
C_{fuel}	fuel costs
$C_{inv,a}$	amortized annual capital cost
$C_{NH_3-H_2}$	The energy conversion of ammonia and hydrogen
C_{rep}	Total Replacement cost
$C_{rep,a}$	Annualized replacement cost
i	interest rate
j	year in the range of system lifetime
$M(CO_2)$	carbon dioxide emission (g)
$M(fuel)_{Powertrain}$	annual fuel consumption of drive system (kg)
$M_{mol(H_2)}$	molar masses of hydrogen (g/mol)
$M_{mol(NH_3)}$	molar masses of ammonia (g/mol)
$M(N_xO)$	nitrogen oxides emission (g)
n	number of years of the loan
$P_{BP\ disch}$	power of discharging
P_E	specific price of electricity

P_E	annual electricity production (kWh)
$P_{EMD-710}$	diesel engine power
P_{fuel}	fuel price
r	annual interest rate
R_t	annual revenue
t	lifespan of the facility (year)

Due to these electrification gaps, transitional solutions need to be implemented, with the favourite proposed solutions being diesel bi-mode and battery electric trains. These have the advantage in that they can use the electrified infrastructure, where possible, but also have the flexibility to reach non-electrified parts of the network. The studies of bi-mode trains show the advantages of lower energy consumption and carbon emissions on discontinuously electrified Great Western Main Line routes for freight (Hoffrichter et al., 2013) and passenger trains (Harrison et al., 2021) in the UK. For most studies of battery-powered trains, the battery pack is used as an energy storage system to store the regenerative or recovered energy (Iannuzzi and Tricoli, 2012). There are a few battery-electric trains (Class 230 powered by Vivarail Battery) (Murray-Smith and Watt, 2020) that have been tested in the UK. These are able to reach a maximum speed of ~ 97 kmph and have a range of 100 km, making them suitable for small branch lines. The study (Popovich et al., 2021) shows that the economic and environmental benefits of converting diesel trains into battery-electric trains by analysing battery price, battery lifetime, battery energy densities, etc (Popovich et al., 2021). However, while exploiting existing infrastructure at low prices, the range and top speed of battery-powered trains are limited due to the low battery capacity.

Fuel cell trains have received increasing attention as they can overcome the low battery capacity and achieve zero emissions during their operation (Hoffrichter et al., 2014; Hoffrichter, Hillmansen and Roberts, 2016; Din and Hillmansen, 2018). Hydrogen fuel cells generate electricity for traction power with only green by-products (waste heat and water), which is ecologically friendly. The UK's first hydrogen-hybrid train (HydroFLEX (Calvert et al., 2021)) operated on the mainline in 2020, with a maximum speed of 160 kmph and a range of up to 480 km. Three recent developments support the UK transition to fuel cell rail: efficient energy management strategy of fuel cell systems, access to green, cheap fuel and reliable support chain, and higher efficient fuel cell.

Many researchers focused on the energy management strategy of a fuel cell battery train. Torreglosa et al. (2014) simulated a hybrid powertrain based on proton exchange membrane fuel cell (PEMFC), battery, and supercapacitor while considering regenerative braking energy. An optimal state machine control strategy has been proposed for fuel cell hybrid tramcar to reduce the hydrogen consumption (Li et al., 2019). In addition to the above energy control strategy, the aging fuel cell and battery degradation are the other key points for fuel cell hybrid train, which limits the lifespan of the powertrains. Deng et al. (2022) used a deep reinforcement learning method to minimise hydrogen consumption and reduce the battery degradation by up to 51% in fuel cell hybrid railway vehicles, which achieve up to 28% improvement in the overall operational cost. A fuel cell multi-mode powertrain model was proposed to show the economic advantages while considering the battery degradation over 40 years (Zhang et al., 2022). Although these fuel cell hybrid trains provide good performance and environmentally friendly solutions, huge challenges, such as robust hydrogen supply chain, safety, and storage space, still remain. Hydrogen storage limits their operation as it does not satisfy their requirements for high power and range, especially for long-distance freight rail.

As a consequence of tackling these challenges, interest in ammonia as a hydrogen carrier and direct fuel for vehicles is gaining momentum (Lan, Irvine and Tao, 2012; Lan and Tao, 2014; Giddey et al., 2017; Cesaro et al., 2021; Royal Society, 2021; Jeerh et al., 2022), because of the following reasons: a) Ammonia is the most extensively used industrial chemical and its annual world production is about 200 million tonnes (Giddey et al., 2017), which is easier to obtain and less expensive to transport than hydrogen; b) Ammonia has 50% more hydrogen by volume than liquid hydrogen when liquefied, making it a desirable choice for storage and transport of hydrogen for hydrogen trains; c) Carbon-free synthesis of ammonia from renewable hydrogen and air-borne nitrogen is possible without the addition of carbon species; d) (Giddey et al., 2017) The price of green ammonia has been projected to fall below $\pounds 0.24/\text{kg}$ (Cesaro et al., 2021), which is 95% lower than green hydrogen (Department for Business, 2021). Therefore, ammonia is a potential fuel for rail applications due to its huge production, high hydrogen density, and reliable supply chain.

As demonstrated by PEM trains mentioned above, PEM fuelled by hydrogen may now be regarded as commercially viable for rail applications (Calvert et al., 2021; Ku, 2021). Ammonia with high storage capacity can also be used as a fuel for PEM. However, ammonia decomposition and purifying techniques are key issues for PEM because of its, according to ISO1468-2 (Halseid et al., 2006; Miyaoka et al., 2018), little tolerance to ammonia (<0.1 ppm). Due to this, ammonia could poison the membrane of PEM (Giddey et al., 2017). Many studies (Alagharu et al., 2010; Lamb, Dolan and Kennedy, 2019; Lucentini et al., 2021; Makhloufi and Kezibri, 2021) have been done to research the ammonia decomposition technology, focusing on membrane reactors systems, catalyst-packed bed membrane reactors, and packed bed membrane reactors. The conversion of these reactors can reach as high as 90%~99% (Itoh et al., 2021), which could satisfy the need for high purity H_2 ($>99.99\%$) for PEM. Giddey (Giddey et al., 2017) mentioned two routes for PEM with ammonia crackers - these have a maximum 15% loss of hydrogen and efficiencies of up to 39%. If the large conversion heat loss of ammonia decomposition could be reutilised (Itoh et al., 2021; Pashchenko and Mustafin, 2022), the efficiency of PEM systems could be improved, which could pave way for rail applications that are fuelled by ammonia.

At the same time, highly efficient solid oxide fuel cells (SOFC) have been utilised as another fuel cell system in numerous recent studies of rail transportation. An integrated direct methane-solid oxide fuel cell powering system (Al-Hamed and Dincer, 2020b) has been proposed, and significant environmental and economic advantages are shown. Seyam et al. (Seyam et al., 2021) compared five alternative fuels (natural gas, methanol, ethanol, dimethyl ether, and hydrogen) for SOFC hybrid rail powertrain and investigated their economic and environmental aspects. Al-Hamed et al. (Al-Hamed and Dincer, 2021) compared the SOFC combined gas turbine with

Table 1
Key parts of five driving systems.

System	Fuel	Cracker	Prime mover	Storage method	Auxiliary power
EMD-710	Diesel	–	Combustion engine	Diesel tank	–
H ₂ -PEM	Hydrogen	–	PEMFC	350 bar CH ₂ vessel ^a	Battery
NH ₃ -SOFC	Ammonia	–	SOFC	ISO tank ^b	Battery
Cracker-PEM	Ammonia	Preheater, reactor	PEMFC	ISO tank ^b	Battery
Cracker-SOFC	Ammonia	Preheater, reactor	SOFC	ISO tank ^b	Battery

^aCalvert et al., 2021; Ku, 2021. ^bElishav et al., 2021.

Table 2
Properties of diesel, hydrogen, and ammonia.

	Density	Hydrogen capacity	LHV	Storage Tank		Prices
	Kg/m ³	wt%	MJ/kg	Pressure bar	Temperature K	£/kg
Diesel	875.00	N/A	43.10	1	300	0.60
Gaseous hydrogen	23.19	5.50	120.10	350	300	1.82 ^a
Ammonia	600.90	17.70	18.80	8–22	233–333	0.11 ^{a,b}

^a Department for Business, 2021.

^b Jackson et al., 2019; Department for Business, 2021.

Alkaline fuel cell fuelled by ammonia, and showed that natural gas and ammonia have more advantages in economic dimensions of the systems when used as transitional fuels to hydrogen. These research only consider SOFC as the auxiliary power system for internal combustion engines, although they show the potentiality of SOFC system as a power-plant for rail transportation.

As the transitional fuel to hydrogen, ammonia has more advantages for SOFC compared to PEM. In ammonia-fuelled PEMFC system, heat exchange is needed to cool the gas from decomposition (450–1000°C) (Li et al., 2013; Rizzuto et al., 2014; Jeerh et al., 2021), in turn, matching the fuel cell operating temperature (67–200°C) (Chandan et al., 2013; Jannelli et al., 2013). However, SOFC can tolerate high temperature fuel and high concentration of ammonia in hydrogen because its operating temperature (700–1000°C) has positive effects on ammonia cracking (Giddey et al., 2017). This means that there is no need to preheat the ammonia or cool the outlet gas from ammonia decomposition for SOFC, which is more energy-efficient than PEM. The energy conversion efficiencies of direct-ammonia SOFC and SOFC with external ammonia crackers could reach up to 52% and 57% (Kishimoto et al., 2020), respectively. These studies identified that the fuel utilisation efficiency of SOFC fuelled by ammonia is much higher than that of diesel engines and PEM. However, the shortage of SOFCs is the high cost which could diminish their benefits. Ammonia-fuelled Fuel cells have many advantages for rail applications, but all of them are limited by their expensive cost and low Technology Readiness Level (TRL).

Most previous studies have not considered ammonia fuelled fuel cells as a power supply system for freight rail transportation. When discussing the economic analysis of powerplant, most researchers think only about the capability of the power systems but not the fuel storage tank and other impacts. This study aims to conduct a technical and economic evaluation of diesel locomotive, PEM, and SOFC systems for freight trains. Specifically, it will evaluate the potential of ammonia-fuelled powertrain systems and the feasibility of ammonia direct SOFC as the powertrain for rail freight. The technical performance is determined by prime mover power, fuel consumption, volume of fuel storage, and CO₂ emissions. The study for economic evaluation is performed utilising fuel cost, LCOE, and discounted payback period. We analyse the sensitivity of the efficiency of cracker and preheater, ammonia price, and carbon tax for these systems.

2. Methodology

The techno-economic analysis examines the systems configurations of the systems, which then serve as the foundation for the models of performance, economy and environment that are used in this study and detailed in this section. Since the performance of rail freight is based on line situation (stops, timetable, and landform), a single run daily is performed. All cases are simulated on a freight line in the UK that runs from Felixstowe South Gbrf to Hams Hall Gbrf. The distance between the two terminals is 318 km, with 6 stops along the way. The freight train has 20 wagon cars with a 1235 tonne capacity.

2.1. Systems configurations overview

The drive-systems for diesel-electric (EMD-710), Hydrogen PEMFC (H₂-PEM), ammonia cracker-PEM (Cracker-PEM), ammonia cracker-SOFC (Cracker-SOFC), and direct ammonia fuelled SOFC (NH₃-SOFC) are illustrated in Appendix. The powertrain systems configurations include fuel storage systems, fuel cell systems, ammonia cracker systems, and prime movers. The key parts (Table 1) of these five driving systems are noted below.

Powertrains, DC-BUS, and Traction Packages are the three main components of all drive-systems, with the Power-Plant part being the most distinguishing feature. The diesel-electric drive system (EMD-710) is modelled as a conventional internal combustion engine

(ICE) delivering power via generator, alternator, and power converters to provide traction to the wheel. In the fuel cell systems (FCS), the PEM and SOFC systems replace the ICE respectively, and the drivetrains transform the electric power into mechanical power via alternators and power converters. The drive systems include the battery for startups, storage of the energy from the fuel cells, and delivering power when the fuel cell power doesn't satisfy the need for traction. The dynamic models can be found in previous works (Hoffrichter et al., 2014; Hoffrichter et al., 2016; Din and Hillmansen, 2018; Calvert et al., 2021).

To meet the demands and constraints that are required of a train on the freight line under investigation, the drive-systems are operated for 6 or more hours a day. The storage systems for all drive-systems are designed in a way such that the diesel and fuel cell systems can operate without refuelling during this single trip. The details of the three fuels are shown in Table 2. Compressed gas hydrogen storage technology (GH2) at 350 bar is commonly applied in drive-systems and has been a subject of research in previous studies (Calvert et al., 2021; Ku, 2021). For rail drive-systems, 350 bar tanks are strongly recommended because of the cheap price (£15.50/kWh (James, 2020)) and sufficient storage space in trains. (James, 2020) The major advantage of H2 over diesel is on account of its lower heating value (LHV) - H2 LHV of 120 MJ/kg embodies 2.8 times more energy than diesel LHV of 43.1 MJ/kg.

For ammonia-fuelled powertrains, ISO containers are used for ammonia storage due to their suitability for long-distance ammonia transportation owing to their low leakage, as was demonstrated by previous leaking safety inspections ISO standards (Elishav et al., 2021). The operating pressure of ISO containers is around 8 – 22 bar and the range of temperatures is 233 – 333 K. Previous studies (Fúnez Guerra et al., 2020) suggest that the cost of small-scale and large-scale ammonia storage is £2.49/kg and £0.56/kg per NH₃, respectively. When liquified, ammonia contains 50% more hydrogen by volume than liquid hydrogen (Royal Society, 2021), making it a safe, practical, and cost-efficient hydrogen storage medium.

The fuel cell prime movers, including SOFC and PEM prime movers, are sized to satisfy the EMD-710 's power requirement at end of life (EoL). This will ensure that the fuel cell prime movers can meet the train's power requirements during its entire lifespan.

The PEM powertrain is adapted from the fuel cell systems being developed for hydrogen-powered trains (Calvert et al., 2021; Ku, 2021). The efficiency of a single PEM cell is around 56% with its performance at EoL being 11% worse than that at the beginning of life (BoL). In PEM prime mover, the coolant sub-system and air sub-system are sized for the whole fuel cell powertrain at rated power, which is powered mainly by the PEM cells.

The electrical output power of a single SOFC is less than 1000 W (Payne et al., 2009), with peak electrical efficiency of 60% whereas the thermal power of this cell is half that of the electrical output power. Due to various challenges, including heat management, durability, and maintenance, there are currently no lab-scale rigs or demonstration plants of SOFCs reaching the MW level. However, to estimate the performance, we assume that an MW scale SOFC stack is constructed in terms of the single cell's performance. The model does not consider the coolant system in SOFC systems due to their high temperature having a positive impact on ammonia decomposition.

Across the entire diesel engine power range, all fuel cell prime movers are more efficient than the diesel engine, with a higher efficiency differential at lower power positions. The SOFC prime mover is the most efficient and keeps stable at 56%, which is 29% higher than the PEM EoL efficiency.

For cracker drive-systems, ammonia is cracked into hydrogen for fuel cell prime movers. The ammonia cracker system is adapted from the ammonia decomposition system for automotive applications (Giddey et al., 2017; Cesaro et al., 2021). The ammonia decomposition system consists of two main elements, a preheater that converts liquid ammonia into gaseous ammonia at a cracking temperature of The 450 °C-1000 °C, and a reactor where the ammonia decomposition occurs. According to Giddey et al. (Giddey et al., 2017; Cesaro et al., 2021), for PEM, 30% of ammonia from the tank is used for preheater and a purifier is also required because an acceptable ammonia concentration in hydrogen is less than 0.1 ppm. Due to the high operating temperature (700–1000 °C), the SOFC systems only use 10% fuel energy (Kishimoto et al., 2020) to slightly heat the ammonia. For direct ammonia-fuelled SOFC, ammonia cracking can occur inside the fuel cell stack over the catalyst anode, with hydrogen being used in the electrochemical reaction, which requires less ammonia for the preheater. In all cracker-powertrains, we assume the efficiency of the reactor is 95%.

2.2. Performance model

The performance metrics are prime movers efficiency, fuel consumption, and fuel storage volume. The powertrains' efficiency is calculated using Eqs. (1–3). For cracker systems, this efficiency ($\eta_{Cracker-PEM}$, or $\eta_{Cracker-SOFC}$) includes the efficiencies of preheater ($\eta_{Preheater-PEM}$, or $\eta_{Preheater-SOFC}$), ammonia cracker ($\eta_{CRACKER}$), and fuel cell (η_{PEM} , or η_{SOFC}).

$$\eta_{Cracker-PEM} = \eta_{Preheater-PEM} \times \eta_{CRACKER} \times \eta_{PEM} \quad (1)$$

$$\eta_{Cracker-SOFC} = \eta_{Preheater-SOFC} \times \eta_{CRACKER} \times \eta_{SOFC} \quad (2)$$

$$\eta_{NH_3-SOFC} = \eta_{Preheater-SOFC} \times \eta_{SOFC} \quad (3)$$

The efficiency of ammonia cracker is decided by the percentage conversion of ammonia ($C_{Cracker(NH_3)}$) and the energy conversion of ammonia and hydrogen ($C_{NH_3-H_2}$).

$$\eta_{CRACKER} = C_{Cracker(NH_3)} \times C_{NH_3-H_2} \quad (4)$$

$$C_{NH_3-H_2} = \frac{\frac{3}{2} \times M_{mol(H_2)} \times LHV_{H_2}}{M_{mol(NH_3)} \times LHV_{NH_3}} \quad (5)$$

$M_{\text{mol}(\text{H}_2)}$ and $M_{\text{mol}(\text{NH}_3)}$ are the molar masses of hydrogen and ammonia, respectively, while LHV_{H_2} and LHV_{NH_3} are the lower heating values of hydrogen and ammonia, respectively.

The annual fuel consumption of the five drive-systems ($M(\text{fuel})_{\text{Powertrain}}$) based on the requirements of diesel engine power ($P_{\text{EMD}-710}$) is defined as:

$$M(\text{fuel})_{\text{Powertrain}} = \frac{\int P_{\text{EMD}-710} dt}{\eta_{\text{Powertrain}} \times LHV_{\text{fuel}}} \quad (6)$$

The calculation of fuel storage volume is based on the fuel consumption and the fuel storage conditions.

2.3. Economic mode

Economic metrics include capital cost, operating and maintenance cost, replacement expenditure, fuel cost, Levelized Cost of Electricity, and discounted payback period. The economic models of the five systems are estimated over the entire 25 years, due to the lifespan of the locomotive of a freight train.

The large capital costs require a loan. Since the lifetime of a locomotive engine is approximately 25 years, the loan is planned for that time. An annual interest rate of 2.5% is considered. The amortized annual capital cost, $C_{\text{inv},a}$, for the investment is estimated as follows:

$$C_{\text{inv},a} = \frac{r(\text{Cap})}{1 - (1 + r)^{-n}} \quad (7)$$

Here r is the annual interest rate, Cap is the capital cost, and n is the number of years of the loan.

The fuel costs (C_{fuel_j}) of five drive-systems considered are calculated using Eq. (8). Supposing the fuel price P_{fuel} changes annually and the price change slope is the same as that in recent decades, the fuel price in the j -th ($Pr_{\text{fuel}}(j)$) year is shown in Eq. (9). As mentioned previously, the fuel prices of the five trains are estimated over the entire 25 years, due to the lifespan of the locomotive of a freight train. Assuming all trains run as planned by using $M(\text{fuel})_{\text{Powertrain}}$ fuel each year, the total cost $C_{\text{fuel}-25}$ of fuel (diesel, hydrogen, or ammonia) in the 25 years is given by Eq. (10).

$$C_{\text{fuel}_j} = Pr_{\text{fuel}_j} \times M(\text{fuel})_{\text{Power-Plant}} \quad (8)$$

$$Pr_{\text{fuel}}(j) = Pr_{\text{fuel}}(t) \times (1 + j \times r) \quad (9)$$

$$C_{\text{fuel}-25} = M(\text{fuel})_{\text{Powertrain}} \times \sum_{j=1}^{25} Pr_{\text{fuel}}(j) \quad (10)$$

Usually, all equipment has an estimated life cycle. On reaching the end of its lifespan, it should be replaced. In this project, the fuel cell prime mover C_{FCrep} , ammonia cracker C_{CRACKER} , and battery are considered. Their costs are summed as C_{rep} in Eq. (11).

$$C_{\text{rep}} = C_{\text{FCrep}} + C_{\text{CRACKER}} + C_{\text{BPrep}} \quad (11)$$

$$C_{\text{CRACKER}} = \frac{\text{InstalledCAPEXofcracker}}{\text{Maximumtractionpower}} \quad (12)$$

The Installed CAPEX of cracker follows a linear relationship with the hourly hydrogen consumption (Cesaro et al., 2021). It can be converted to a new indicator, which is expressed as follows in Eq.12. In this study, the maximum traction power is used as the denominator in all estimates and analyses. The values of C_{FCrep} and C_{CRACKER} are obtained using the relevant references, as will be seen in the next section.

The battery pack needs to be replaced due to its degradation. Every time it charges or discharges, the degradation effect of the materials would reduce the battery capacity. If the maximum capacity decreased to approximately 75%, it would be considered failed.

$$C_{\text{BPrep}} = C_{\text{BP}} \times \left(\frac{\int \frac{P_{\text{BP}_{\text{disch}}}}{C_{\text{apBP}}} dt}{DOD_{\text{lifespan}}} - 1 \right) \quad (13)$$

$P_{\text{BP}_{\text{disch}}}$ is the power of discharging, C_{apBP} is the battery capacity, and DOD_{lifespan} is the depth of discharge (Zhang et al., 2022).

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

$$C_{\text{rep},a} = \frac{i \cdot (1 + i)^n}{(1 + i)^n - 1} \cdot \frac{C_{\text{rep}}}{(1 + i)^t} \quad (14)$$

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

The levelized cost of electricity (LCOE) is calculated as:

$$LCOE = \frac{\text{TotalCosts}(\pounds)}{\text{AnnualElectricityProduction}(kWh)}$$

Table 3Well-to-tank carbon dioxide equivalent factors (CEF_{WTT}) and tank-to-wheel carbon dioxide equivalent factors (CEF_{TTW}) for different fuels.

Fuel type		Well-to-tank (CEF_{WTT}) g CO ₂ e/MJ	Tank-to-wheel (CEF_{TTW}) g CO ₂ e/MJ
Diesel		85.00 ^a	454.03
Brown ammonia (BrA)	Natural gas	138.29 ^b	N/A
Blue ammonia (BA)	Natural gas with carbon capture and storage	61.70 ^b	N/A
Green ammonia (GA)	Nuclear-powered or renewable ammonia production	5.80 ^c	N/A
Blue hydrogen (BH)	Natural gas with carbon capture and storage	227.60 ^d	N/A
Green hydrogen (GH)	Electrolysis, electricity from wind energy	3.60 ^d	N/A

^a Hoffrichter et al., 2012.^b Lee et al., 2022.^c Al-Aboosi et al., 2021.^d Prussi et al., 2020.

$$= \frac{C_{inv,a} + C_{rep,a} + C_{O\&M,a}}{E_{electricity}} \quad (15)$$

The Discounted Payback Period (DPP) is the period (in years) required to recover the initial investment through the cash inflow given by the power systems (considering money discount). The Discounted cash flows (DCF) and DPP are calculated as the year at which the following equation is satisfied:

$$DCF = \sum_{j=1}^{DPP} NAI_j - C_{inv} \quad (16)$$

The Net Annual Income ($NAI_{j=1,n}$, the index j is the year in the range of system lifetime) for each power system is calculated by means of the following equation:

$$NAI_j = \frac{R_j - C_{O\&M_j} - C_{rep_j} - C_{fuel_j}}{(1+i)^j} \quad (17)$$

The annual revenue, R_j , is given by:

$$R_j = p_E \bullet P_{Ej} \quad (18)$$

where p_E is the specific price of electricity, while P_{Ej} is the annual electricity production (kWh).

2.4. Environmental model

Environmental impacts are also important for zero-emissions trains. This environmental analysis is based on the well-to-wheel (WTW) carbon dioxide equivalent (CO_2e) emissions. The WTW has two carbon footprints: well-to-tank (WTT) and tank-to-wheel (TTW). The formula to estimate the CO_2 equivalent emissions is:

$$CO_{2e_{WTW}} = CVF \times (CEF_{WTT} + CEF_{TTW}) \quad (19)$$

CVF is the calorific value of fuel, CEF_{WTT} is well-to-tank carbon dioxide equivalent factor for the fuel, CEF_{TTW} is tank-to-wheel carbon dioxide equivalent factor for the fuel.

Since hydrogen and ammonia are carbon-free molecules, their TTW carbon footprint is disregarded compared to their WTT footprint. Their CEF_{WTT} is shown in Table 3. The emissions of diesel prime mover include CO_2 and N_xO . The tank-to-wheel carbon dioxide equivalent factor of diesel prime mover ($CEF_{TTW(Diesel)}$) is calculated by the following formulas:

$$CEF_{TTW(Diesel)} = \frac{CO_{2e_{EMD-710}}}{CVF_{EMD-710perday}} \quad (20)$$

$$CO_{2e_{EMD-710}} = M(CO_2) + 298 \times M(N_xO) \quad (21)$$

The $M(CO_2)$ and $M(N_xO)$ are, according to the emission of EMD-710, at different Notch positions (Christopher Frey and Rastogi, 2018).

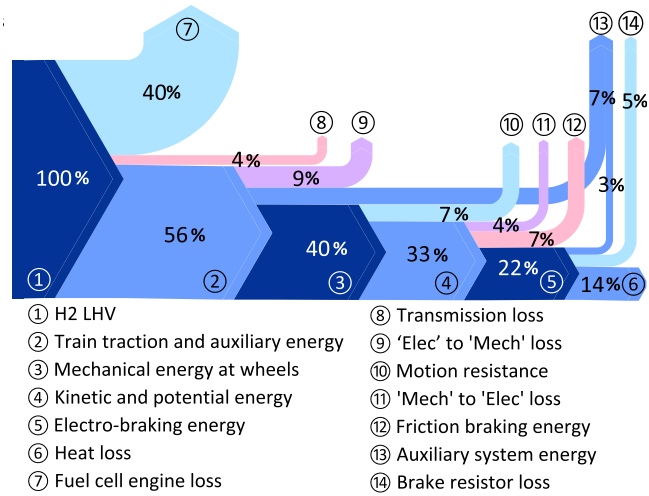


Fig. 1. Sankey diagrams for the H2-PEM train system.

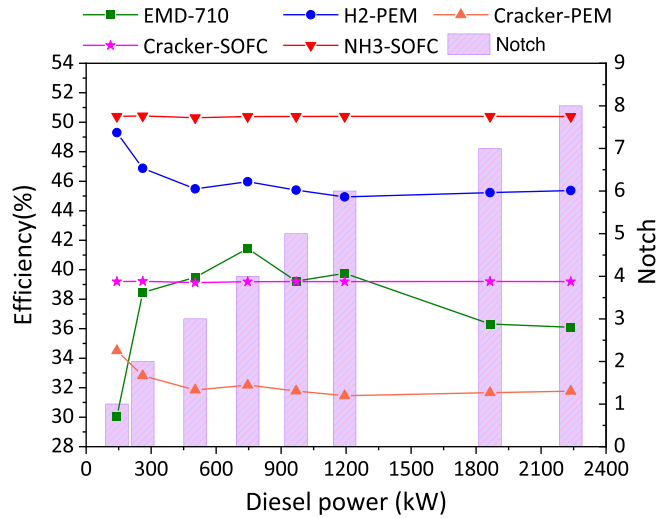


Fig. 2. Powertrain efficiencies of different cases.

3. Case study

In this section, energy consumption and environmental impact of the five drive-systems (EMD-710, H2-PEM, Cracker-PEM, Cracker-SOFC, and NH3-SOFC) are evaluated using the aforementioned methodology.

3.1. Energy consumption

To study the energy efficiency of the whole system of the rail freight, the H2-PEM energy consumption components with measured and estimated proportions, based on previous studies (Hoffrichter et al., 2016; Tian et al., 2017), are illustrated in Fig. 1. The train traction and auxiliary energy flows for each driving system are straightforward and similar to H2-PEM. The greatest portion of fuel energy is wasted in prime mover loss – PEM system at 40% loses less energy than the diesel system at 55–70%. As shown in Fig. 1, auxiliary systems require a significant portion of the total energy. Heat loss from braking is another major share of the fuel energy that is not regenerated in these driving systems.

The powertrain efficiency is determined by the prime mover and drivetrain efficiencies, which affect the final fuel consumption (Hoffrichter et al., 2016). The efficiency versus power of a Class 66 locomotive based on six different powertrain configurations is shown in Fig. 2. Each curve is plotted according to the eight Notches of the diesel engine (EMD-710). The SOFC and PEMFC systems are sized to satisfy the power requirements in terms of their EoL performance. The efficiencies of the cracker and preheater are included for the systems utilising onboard ammonia cracker.

Table 4
Comparison of powertrain efficiencies.

	Prime mover	Fuel	Type	Powertrain efficiency	Ref.
EMD-710	ICE	Diesel	Freight	35%	This study
	ICE	Diesel	Passenger	33%	Al-Hamed and Dincer, 2021
	ICE	Diesel	Freight	40%	Hoffrichter, Hillmansen and Roberts, 2016
		Electricity			
H ₂ -PEM	PEMFC	H ₂	Freight	45%	This study
Cracker-PEM	PEMFC	NH ₃	Freight	32%	This study
	PEMFC	H ₂	Freight	40%	Zenith et al., 2020
	PEMFC	H ₂	Passenger	43%	Calvert et al., 2021
	PEMFC	H ₂	Passenger	28%	Al-Hamed and Dincer, 2021
NH ₃ -SOFC	SOFC	NH ₃	Freight	52%	This study
Cracker-SOFC	SOFC	NH ₃	Freight	39%	This study
	SOFC + hybrid	Natural gas	Passenger	61%	Al-Hamed and Dincer, 2020c)
	SOFC + hybrid	Methane	Passenger	79%	Al-Hamed and Dincer, 2020a
	SOFC + hybrid	NH ₃	Passenger	71%	Al-Hamed and Dincer, 2019
	SOFC + hybrid	Natural gas	Passenger	67.8%	Al-Hamed and Dincer, 2021

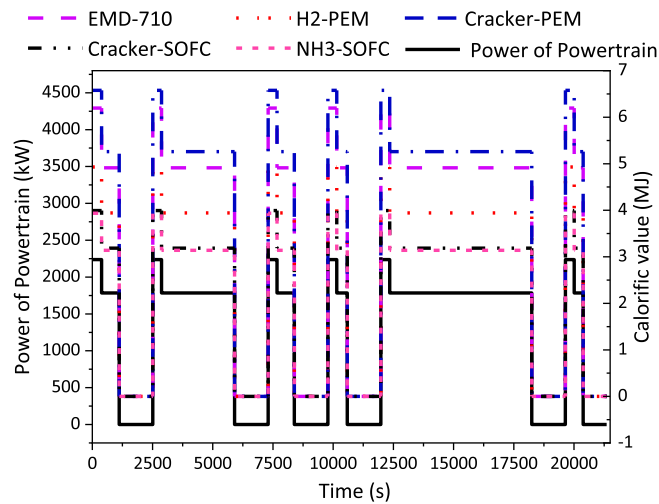


Fig. 3. The power demand profile of the case route and the prime energy from fuel tanks of five cases.

At Notch 7 and 8 positions, NH₃-SOFC efficiency (52%) is best, whereas Cracker-PEM efficiency is the lowest. Although there are slight fluctuations at Notches 1, 2, and 3, the efficiencies of all systems are stable at high Notches. Due to heat loss from ammonia decomposition, the powertrain systems with crackers are all 13% less efficient than the direct fuel powertrains.

The diesel engine EMD-710 has powertrain efficiencies ranging from 30% to 41% across all the notches. The H₂-PEM could increase these efficiencies by 10%–20% of the original value, depending on the notch investigated. Table 4 provides a comparison of powertrain efficiency against other cases. Studies conducted on PEMFCs show that hydrogen-fueled passenger rails have 20% higher efficiency than diesel ones, confirming our estimate. The higher powertrains' efficiencies contribute to less energy consumption and higher power at wheels (Calvert et al., 2021). Therefore, PEMFs provide an efficient solution that is a viable alternative to both diesel and diesel-electric powertrains.

Due to single SOFC efficiency (Payne et al., 2009) being 11% higher than the single PEM fuel cell (Cano et al., 2018), the Cracker-PEM efficiency is 5% lower than the Cracker-SOFC. Recent studies also found that the direct-fueled SOFC powertrain is around 10% more efficient than the PEMFC powertrain, in line with the results of our research (as shown in Table 4). Furthermore, rail powertrain energy efficiency of 61%–79% could be achieved when it is integrated with hybrid-SOFCs - leading to SOFC showing the potential of being the most efficient rail powertrain.

Ammonia has the potential to be a direct fuel for fuel cell powertrains. Al-Hamed et al. (Al-Hamed and Dincer, 2020a, 2020b, 2020c, 2020d) designed an integrated system with a direct ammonia-fuelled alkaline fuel cell (AFC). During these studies, researchers achieved an energy efficiency of 42%. Our estimate of direct ammonia fuel cell (NH₃-SOFC) is 10% more efficient than the AFC powertrain, as well as 13% more efficient than the Cracker-SOFC powertrain. Benefiting from the high operating temperature of the SOFC, ammonia as a direct fuel is more efficient for this drive-system as opposed to the other ones.

The energy consumed by the five powertrains for our freight line has been estimated using a complete model of the hybrid powertrains published in the past (Hoffrichter et al., 2016). (Hoffrichter et al., 2016) As shown in Fig. 3, the power of the powertrains varies from 1784 kW to 2237 kW per day.

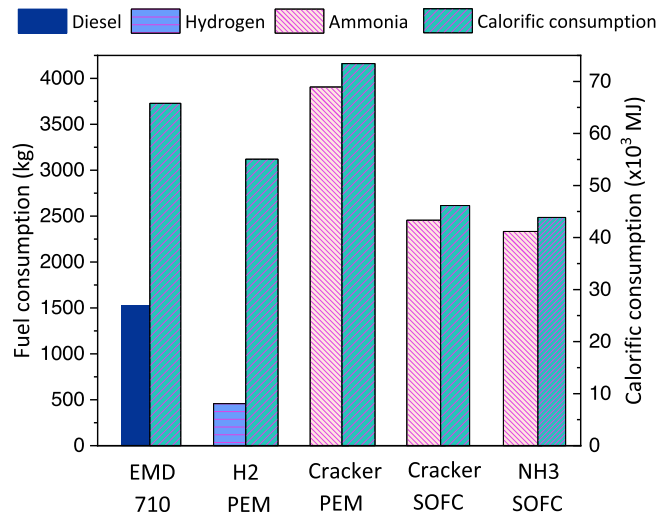


Fig. 4. Fuel consumption along the track per day.

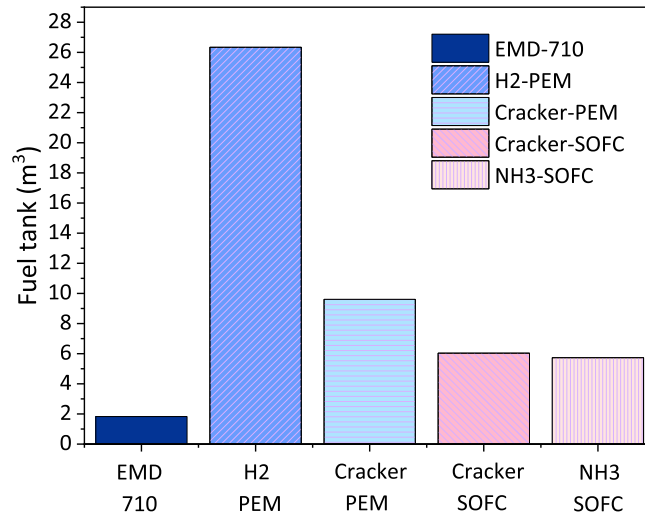


Fig. 5. Comparison of the storage tank sizes.

Reducing fuel consumption is an important contribution to the lower cost of the train power systems. According to the efficiency of five powertrains (Fig. 2) and Eqs (1–3), the fuel consumption for each was calculated. In Fig. 3, the consumption of diesel, hydrogen, and ammonia is compared based on calorific values versus time. Due to the lower engine efficiency and significant heat loss in the cracker, the Cracker-PEM uses the most fuel (5.26–6.57 MJ). For the SOFC powertrains, the high efficiency of the SOFC prime mover and low heat losses during ammonia decomposition contribute to the lowest consumption of calorific values (3.2–3.9 MJ).

The daily consumption of ammonia, hydrogen, and diesel is shown in Fig. 4. In terms of fuel weight, the H2-PEM has the lowest fuel consumption (458 kg per day). This is as a result of the much higher low heating value of hydrogen per kilogram of hydrogen compared to diesel or ammonia. For the ammonia-fuelled fuel cell powertrains, Cracker-PEM requires 1451 kg and 1574 kg more ammonia than the Cracker-SOFC (2455 kg per day) and NH3-SOFC (2333 kg per day), respectively. This is due to the low PEM efficiency and 20% more ammonia than SOFC for the preheater. The energy consumed by SOFC freight trains might increase because of the additional fuel weight but they still have around 20% less calorific consumption than EMD-710 owing to the high efficiency of SOFC. However, compared to battery freight trains (Zenith et al., 2020), fuel cell freight trains have more calorific consumption due to their 40% heat loss.

The fuel storage of the five drive-systems is plotted in Fig. 5. The EMD-710 only requires 1.74 m³ to store the diesel due to its high density of 875 kg/m³. Hydrogen is stored in 350 bar GH₂ vessels (Calvert et al., 2021) and at normal temperature with a density of about 23.19 kg/m³, this resulting in the largest volume of the fuel at 26.30 m³ for a single trip. Consequently, like with electric powertrains, extra wagons will be required for hydrogen tanks in the freight trains but the energy density of a hydrogen wagon is over 12 times greater than that of a battery wagon (Hoffrichter et al., 2016). In terms of storage space, the ammonia-fuelled trains have the

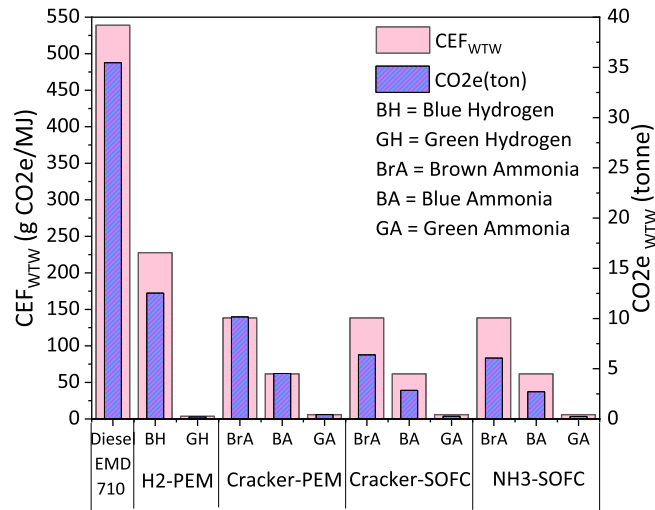


Fig. 6. WTW carbon emission of five cases per day.

advantage over the hydrogen-powered system. The ammonia is stored in an ISO tank at 18 bar and 300 K with a density of about 601 kg/m³. The Cracker-PEM could reduce 63% of storage space compared to H2-PEM. For the ammonia-fuelled power systems, the Cracker-PEM requires the largest storage volume (9.60 m³) due to its low efficiency and huge ammonia consumption. However, the required volume is not large enough to be an issue in ammonia-fuelled trains.

3.2. Emissions

The primary benefit of fuel cell powertrains is the consumption of clean fuels without any direct CO₂e emissions. Out of the five systems, CO₂ and NO_x are only emitted by EMD-710 – it produces 84 kg NO_x and 4710 kg CO₂. The CO₂e_{WTW} can be calculated according to Eqs. (19)–(21). As shown in Fig. 6, EMD-710 has the highest carbon emissions. Train systems utilising green fuel produce the lowest carbon emissions because the production of these fuels is from renewable energy. Brown ammonia-fuelled trains could reduce carbon emissions by 66% compared to EMD-710 but they cannot get zero carbon emissions.

From Table 3, diesel has the lowest carbon emissions in well-to-tank, but it produces the most CO₂e in tank-to-wheel. Compared to the zero-emission fuel cell powertrains, the ICE with diesel has worse effects on the environment in transportation applications (Al-Hamed and Dincer, 2021). Al-Hamed et al (Al-Hamed and Dincer, 2021) estimated that the carbon emissions of diesel trains are higher than that of natural gas, ammonia, and hydrogen trains per duty cycle. However, the WTW carbon emissions are not considered in their analysis. In other railway WTW carbon emission analysis (Hoffrichter et al., 2012), diesel and ICE trains also produce three times more carbon emissions than gas hydrogen fuelled-fuel cell trains, in line with our analysis. The environmental analysis of different fuels for trains indicates that ammonia and hydrogen are environmentally friendly fuels for transportation applications.

4. Results and discussions

This section presents and discusses the comparison results of five powertrains for rail freight applications. Economic analysis, and sensitivity analysis are performed using the methodology defined in the previous section. The sensitivity analysis focuses on the fuel price, carbon tax, the efficiency of ammonia cracker and preheater, and the battery.

4.1. Economic analysis

The economic analysis investigates fuel cost, CAPEX (Capital Expenditure), OPEX (Operational Expenditure including the maintenance costs, 'O&M'), REPLEX (Replacement Expenditure), LCOE (Levelized Cost of electricity), and discounted payback period. The single-variable LCOE sensitivity analyses are carried out, including the efficiency of cracker and preheater, ammonia price, and carbon tax.

In UK, the freight trains run on red diesel (GOV.UK, 2021). From 2010 to 2022, red diesel prices in the UK increased from £0.553 per litre to £0.791 per litre (AHDB, 2023). The average yearly rate of increase is 2.2% (AHDB, 2023). Furthermore, the hydrogen price has also risen 2.2% per year according to the 2015–2050 forecast of hydrogen cost for the UK (Steinberger-Wilckens et al., 2017; Zhang et al., 2022). A combination of Carbon Capture, Usage and Storage (CCUS), and methane reformation in the UK resulted in a cost of green hydrogen ranging from £1.60/kg to £2.83/kg (Jackson et al., 2019; Department for Business, 2021) in 2021. The brown ammonia price rose from £0.149/kg in 2001 to £0.265/kg in 2021 (Nutrien. Nutrien fact book 2019; 2019, 2019), whereas electricity prices rose about 3.7% per year since 2000 (GOV.UK, 2022). To unify the start year of each type of energy price change rate, the energy

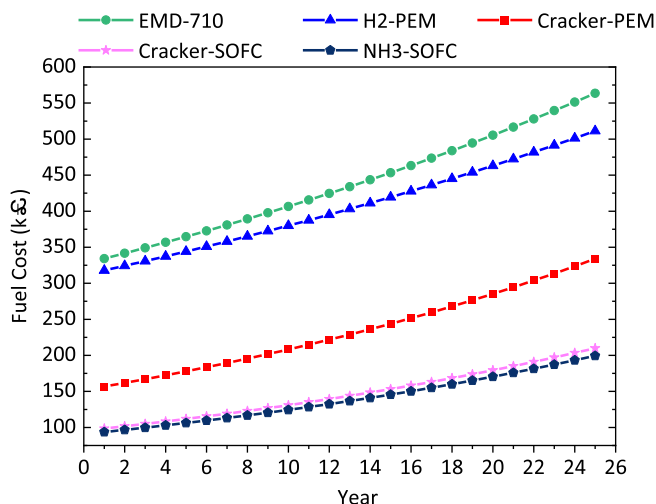


Fig. 7. Fuel cost of five power systems in 25 years.

Table 5
CAPEX.

System	Prime mover (£/KW)	Cracker (£/KW, ton H ₂ /hr)	Installation (£/KW, % of Prime mover)	Fuel Tank (£/ m ³)	Total CAPEX (k£/kW)
EMD-710	750.00	–	75.00 (10.0%)	800.00 ^a	737.36
H ₂ -PEM	830.00 ^b	–	187.58 ^b (22.6%)	10,043.00 ^{c,d}	1,135.74
NH ₃ -SOFC	7,853.38 ^e	–	1,774.86 ^e (30.0%)	1,802.70 ^f	9,367.56
Cracker-PEM	830.00 ^b	965.56 ^g (0.076 ton H ₂ /hr)	187.58 ^b (22.6%)	1,802.70 ^h	2,020.10
Cracker-SOFC	4,150.00 ⁱ	823.92 ^g (0.062 ton H ₂ /hr)	937.90 ⁱ (30.0%)	1,802.70 ^j	5,775.66

^a Ahluwalia et al., 2022. ^b Deloitte, 2021. ^c James et al., 2016. ^d Apostolou, 2021. ^e Minutillo et al., 2021. ^f Nayak-Luke et al., 2021. ^g Cesaro et al., 2021. ^h Nayak-Luke et al., 2021. ⁱ Ammermann et al., 2015. ^j Nayak-Luke et al., 2021.

Table 6
O&M, REPLEX.

	Description	Lifetime (years)	O&M,a (£/KW, %)	REPLEX (£/kW-10yrs, %)
EMD-12-710G3	EMD-710	25	3.23 ^a (0.43%)	
PEMFC	H2-PEM	10	42.33 ^b (5.10%)	40.09 ^b (4.83%)
	Cracker-PEM			
SOFC (NH ₃)	NH ₃ -SOFC	10	431.94 ^c (5.50%)	3,366.74 ^d (42.87%)
SOFC (H ₂)	Cracker-SOFC	10	228.25 ^d (5.50%)	1,779.11 ^d (42.87%)
Ammonia Cracker	Cracker-PEM	10	9.66 (1.00%)	724.17 (75.00%)
	Cracker-SOFC		8.24 (1.00%)	617.94 (75.00%)

^a TNO (Netherlands Organization for Applied Scientific Research), 2018. ^b Deloitte, 2021. ^c Minutillo et al., 2021. ^d Ammermann et al., 2015.

base price is chosen from 2021. The prices of the fuels can be seen in Table 2. It is assumed that diesel, electricity, hydrogen, and ammonia prices have increased at yearly rates of 2.2% (AHDB, 2023), 3.7% (GOV.UK, 2022), 2% (Steinberger-Wilckens et al., 2017; Zhang et al., 2022), and 3.2% (Nutrien. Nutrien fact book 2019; 2019, 2019), respectively. Following this increasing tendency, the price of hydrogen, ammonia, and diesel in 25 years would reach £3.05/kg, £0.23/kg and £1.01/kg.

The fuel costs of the five systems are shown in Fig. 7. Although diesel fuel is currently much cheaper than hydrogen, the fuel cost of

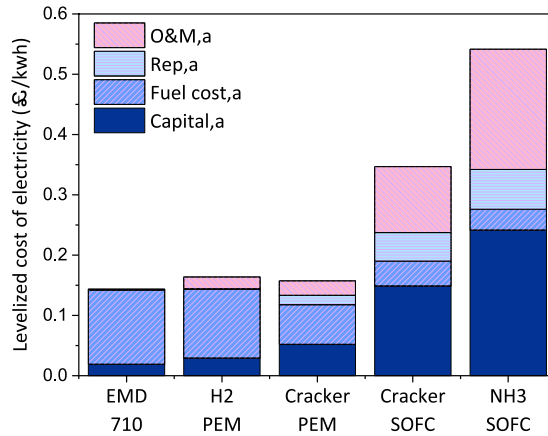


Fig. 8a. Levelized cost of electricity.

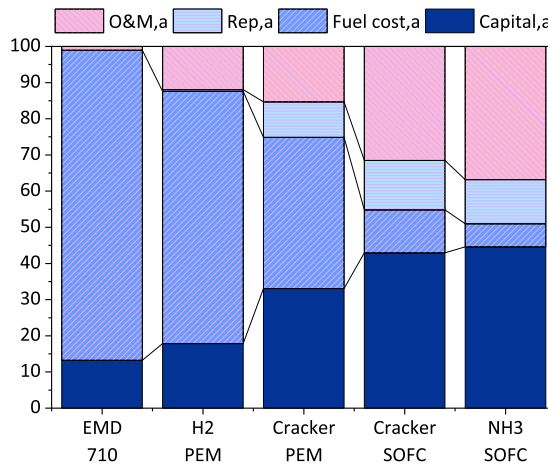


Fig. 8b. Levelized cost of electricity.

‘EMD-710’ is still higher than ‘H2- PEM’ due to the higher heating value of hydrogen and higher energy efficiency of fuel cell technology. All ammonia-fuelled power systems have low fuel costs over the estimated 25 years due to the favorable ‘brown’ ammonia price now. If hydrogen powered trains use ammonia as a hydrogen carrier (Cracker-PEM), the fuel cost could drop by around 40% compared to direct hydrogen fuelled train (H2-PEM). The SOFC trains have the lowest fuel cost due to their high-power generation efficiency and lower heat loss. The fuel cost of Cracker-SOFC and NH3-SOFC follows the same increasing trend over the 25 years owing to their same fuel and small calorific consumption difference.

Tables 5 and 6 show the CAPEX (Capital Expenditure), the OPEX (Operational Expenditure including the maintenance costs “O&M”), and the REPLEX (Replacement Expenditure) of the five systems in comparison. The CAPEX includes initial cost elements such as prime mover technologies, ammonia crackers (if needed), installation costs, and fuel tanks. The O&M costs over 25 years exclude the common cost elements such as labour, insurance, and other attachments. Fuel cell and cracker cases include the REPLEX due to their relatively short 10-year lifespan. The durability of the SOFCs fed by ammonia is still under testing but experiments demonstrate that no severe changes or deterioration to cell performance are observed after long operation periods. The ammonia crackers for rail and marine are still on lab-scale but the ammonia transportation technology is developed, and it has the potential to be considered as a part of the power plant for rail.

The breakdown and evaluation of LCOE (£/kWh) are presented in Fig. 8(a)(b). The LCOE is dominated by fuel costs except in the SOFC cases. The diesel train is the most cost-effective drive-system because of its high TRL, low O&M, and no replacement cost. This forecast matches the existing estimate (Zhang et al., 2022). As shown in Figs. 8(b), 10 % more O&M is needed in Cracker-PEM because of the huge cost of cracker CAPEX and its REPLEX. However, Cracker-PEM still has a more economic advantage due to the lower fuel cost. The SOFC trains are not competitive in the LCOE. Nonetheless, reducing SOFC CAPEX by 60% in 2030 (Europe J P I U, 2019) could make it cost-competitive with EMD-710 and H2-PEM. The reader should note that these results do not consider the revenue coming from the sales of heat and braking power to the grid, which could be reutilised in the locomotive and other auxiliary systems.

Considering the price change over the entire 25 years, the discounted payback period (DPP) is predicted in Fig. 9. In this analysis,

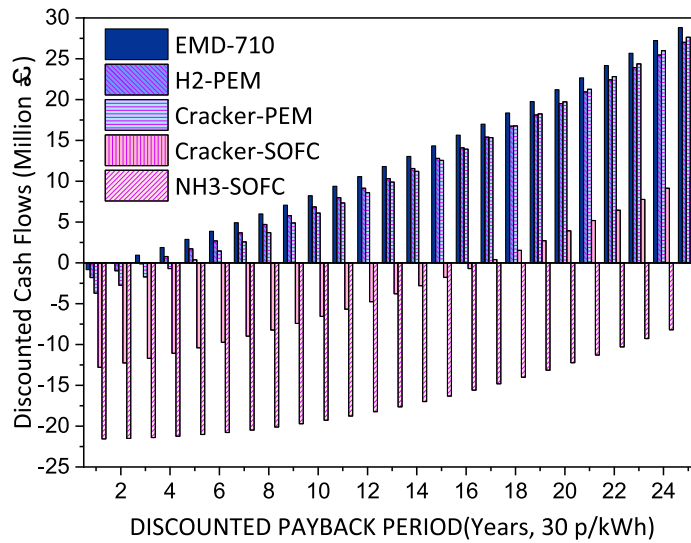


Fig. 9. Discounted payback period.

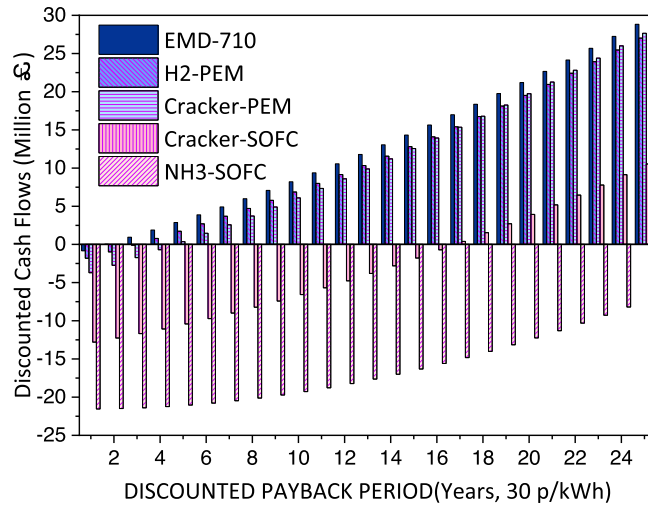


Fig. 10. Sensitivity of the Ammonia price on the fuel costs.

Table 7
LCOE sensitivity limits.

	Lowest estimate	Ref.	Highest estimate	Ref.	Unit
Diesel price	0.60	(BoilerJuice, 2023)	1.30	(BoilerJuice, 2023)	£/kg
Hydrogen price	1.82	Blue hydrogen (Department for Business, 2021)	5.36	Green hydrogen (Department for Business, 2021)	£/kg
Ammonia price	0.11	Brown ammonia (Jackson et al., 2019; Department for Business, 2021)	1.00	Brown ammonia (Philibert, 2017)	£/kg
CO _{2e} price	2	(European Union Emissions Trading System, 2023)	90	(Offer et al., 2011; European Union Emissions Trading System, 2023)	£/ton
Preheater	10	(Giddey et al., 2017; Cesaro et al., 2021)	30	(Giddey et al., 2017; Cesaro et al., 2021)	%
Cracker efficiency	90	(Giddey et al., 2017; Cesaro et al., 2021)	100	(Giddey et al., 2017; Cesaro et al., 2021)	%

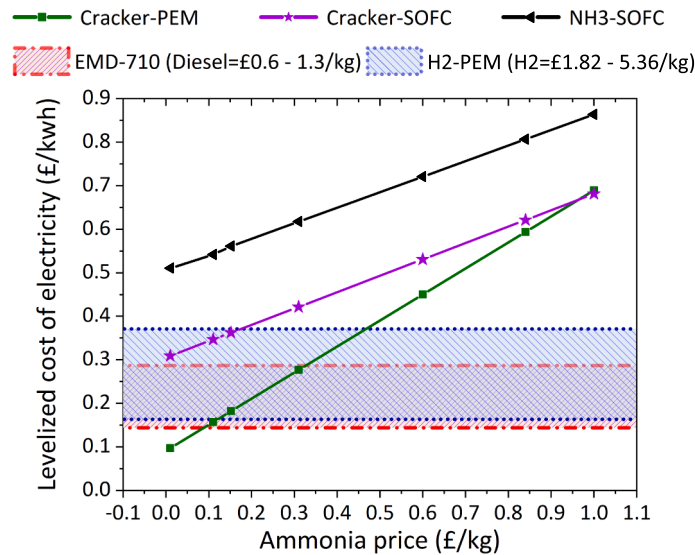


Fig. 11. The effect of ammonia price on the levelized cost of electricity.

the revenues from the selling (use) of electricity have been taken into consideration. The electricity price used in the study is £0.3/kWh (Department for Business, 2021), and the price change over the entire 25 years is also considered.

The DPP of the ‘Cracker-PEM’ and ‘H2-PEM’ is shorter than 5 years, which is commensurate with the international estimate (Zenith et al., no date). The discounted cash flow of Cracker-PEM exceeds the H2-PEM after 18 years due to the high-interest rate of hydrogen price. The Cracker-SOFC is more competitive than the NH3-SOFC, which is due to the relatively inexpensive direct hydrogen-fuelled SOFC. The NH3-SOFC case cannot make economic sense over 25 years according to its current annual cost.

4.2. Sensitivity analysis

Single-variable sensitivity analysis of the five drive systems is analysed in this study, including ammonia price, carbon tax, the preheater, and cracker efficiency. Table 7 shows the low and high estimates for this sensitivity analysis.

The cost of the five train systems is dominated by the fuel cost, according to the breakdown of LCOE. Therefore, prices of diesel, hydrogen, and ammonia generate the most unpredictability. The economics of hydrogen production are still the main challenge in using hydrogen as a fuel for transportation applications (Sharma and Ghoshal, 2015). The red diesel price has had small fluctuations and low cost for last four years (BoilerJuice, 2023). The blue and green hydrogen price is more expensive than red diesel. According to the existing estimate (Al-Hamed and Dincer, 2021; Herwartz et al., 2021), the green hydrogen is only a financially viable fuel for trains if the price per kilogram is less than £1.90 (Al-Hamed and Dincer, 2021).

Compared to hydrogen, cheaper ammonia is a feasible alternative fuel. The economics of ammonia production are dominated (70–90% (Jackson et al., 2019)) by feedstock costs; therefore, the potential for ammonia as a hydrogen carrier is strongly dependent on the economics of manufacturing the necessary hydrogen feedstock in regions where low/zero-carbon hydrogen will be accessible and transporting it to the UK. Data over the last 5 years suggests that ammonia from US Gulf Coast and the Middle East is much cheaper than that in Europe (Philibert, 2017; Makhoulfi and Kezibri, 2021).

Figs. 10 and 11 illustrate the impact of ammonia price on total fuel costs and LCOE. Total fuel costs have inflection points when the price of ammonia is between £0.20/kg and £0.55 /kg, depending on the diesel and hydrogen price at that time. Compared to the ‘H2-PEM’ system, with no cracker fuel loss and high calorific value of hydrogen, the ammonia-fuelled cases face a stringent price range. However, the ammonia-fuelled cases have a clear advantage when they are compared with highest fuel price hydrogen-fuelled case. Ammonia-powered trains only lose their fuel price advantage when the price of ammonia reaches £0.55/kg. As with other estimates (Al-Hamed and Dincer, 2021), the total fuel cost of the hydrogen-powered trains could be seven times higher than that of ammonia-fuelled trains if green hydrogen is used. For the SOFC system, the total fuel cost is always lower than the EMD-710 and H2-PEM at the highest fuel price. Fuel prices also affect the LCOE seen in Fig. 11, which considers other costs. The cases with cracker make more economic sense compared to ‘EMD-710’ with most expensive diesel price.

The carbon tax is the next important factor to influence the economics, especially for ‘EMD-710’. A scenario study is carried out here to gauge the impact brought by the introduction of the carbon tax in the coming years. Only the carbon or other gaseous (NOx) emissions from the locomotive are considered, this study excludes fuel production and transport or any auxiliary system emissions (Brandon and Kurban, 2017).

Globally, a wide range and diversity of carbon pricing schemes are coming into force. Although the introduction of the reserve has helped stabilise the EUA price in 2019, there was a one-third price drop in 2020 because of the COVID-19. However, in line with the

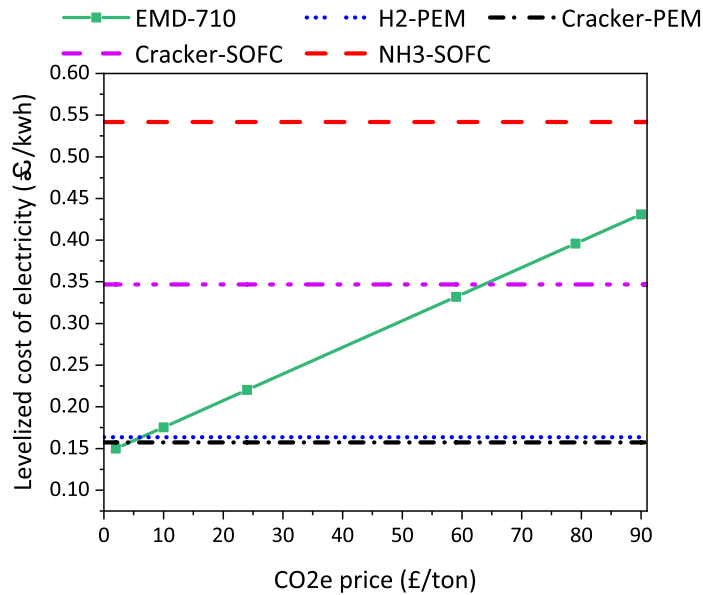


Fig. 12. The effect of the carbon tax on the levelized cost of electricity.

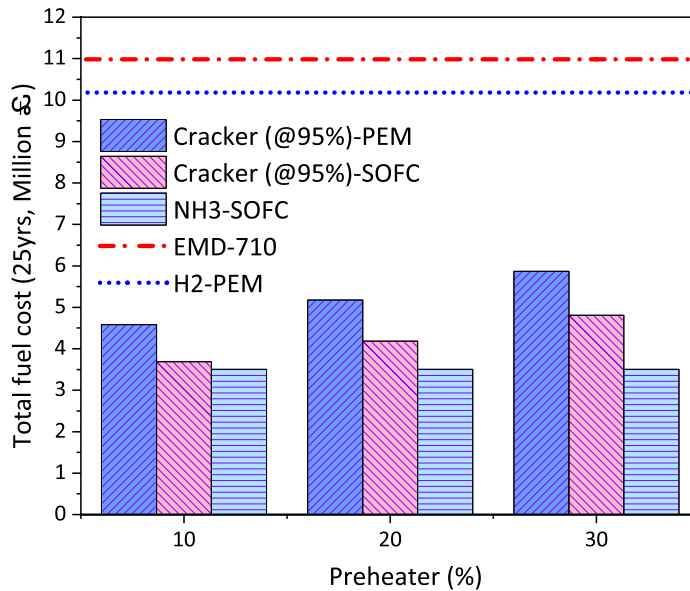


Fig. 13. Sensitivity of the proportions of the fuels used in the preheater. ('Cracker-PEM' and 'Cracker-SOFC' at cracking efficiency of 95%, 'NH3-SOFC' at 100%).

European Union’s commitment to become carbon-neutral by 2050 and a study by the World Bank, the carbon price is predicted to rise annually (World Bank, 2020). In light of this projected trend in future carbon prices, a sensitivity analysis has been conducted.

In Fig. 12, NH3-SOFC has the highest LCOE at all times. The carbon tax would cause the 'EMD-710' case to lose its economic advantage to the 'H2 PEM' from £5/t. Cracker-SOFC is cost-competitive compared to EMD-710 when a moderate carbon tax price of £65 /t CO2e starts to be implemented. The cost savings of fuel cell trains compared to diesel trains are considerably greater when the carbon tax is included (Offer et al., 2011; Al-Hamed and Dincer, 2021). Saving of 27% could be achieved for hydrogen hybrid vehicles compared to ICE vehicles when considering the £90/ton carbon tax in the UK (Offer et al., 2011). For freight trains in this study, 67% saving could be achieved, which reveals that fuel cell has the potential to be used in rail powertrain.

Ammonia decomposition is achieved using ammonia crackers and requires high temperatures of 450 °C to 1000 °C to ensure complete NH3 conversion. However, the performance of the cracker and preheater can be influenced by different decomposition catalysts and improved by utilizing a thermochemical waste-heat recuperation system (Pashchenko and Mustafin, 2022),

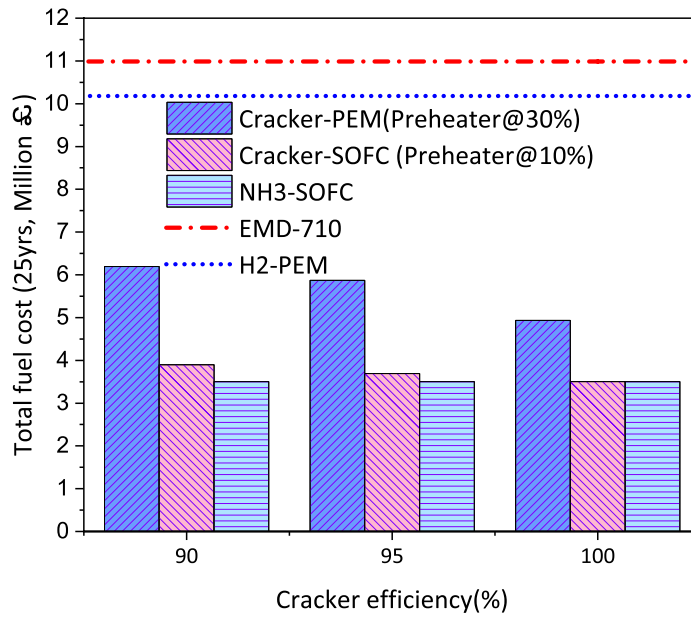


Fig. 14. Sensitivity of the cracker efficiency. (The preheater fuel consumption of ‘Cracker-PEM’ and ‘Cracker-SOFC’ is 30% and 10% of total fuel input, respectively).

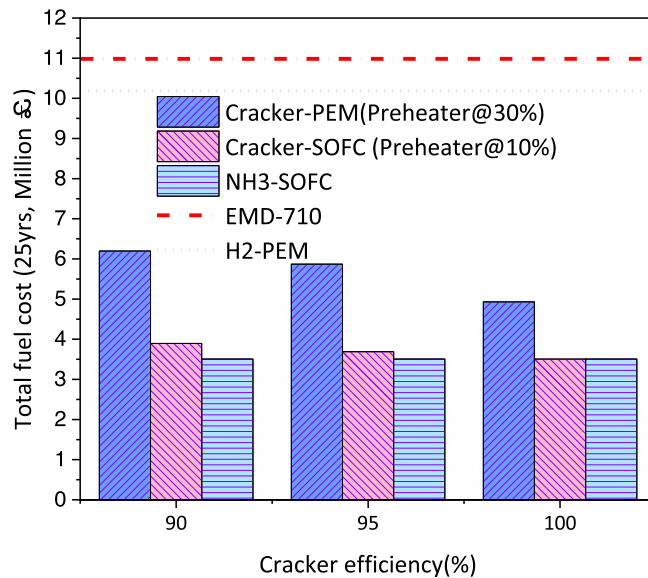


Fig. 15. Sensitivity analysis of LCOE for NH3-SOFC based on low and high values for key model inputs.

respectively, which can result in differences in the cracking efficiency and fuel consumption of the preheater (Giddey et al., 2017; Cesaro et al., 2021). These factors can influence the LCOE, and the limits of their estimated parameters are shown in Table 7. As shown in Fig. 13, the use of more ammonia for preheating increases fuel use, which in turn raises fuel prices. By reducing energy loss in the ammonia cracker, a high cracking efficiency can be attained – Fig. 14 shows cracking efficiencies.

The single-variable LCOE sensitivity analyses of NH3-SOFC and H2-PEM are carried out. The change rate of NH3-SOFC sensitivity parameters is changed based on that of EMD-710 and H2-PEM, and the forecast from IEA. These realistic and applicable parameters are used to estimate the competitiveness of SOFC in comparison to other cases. The same methodology is applied to the sensitivity analysis of PEMFC (refer to Fig. 16(a)). In Fig. 16(b), the same change rate is chosen, which is determined to be the most influential factor. Fig. 15 and Fig. 16(a), (b) indicate that fuel price affects both SOFC and PEM systems. The LCOE of NH3-SOFC increased by ~ 59% if the ammonia price rose to 1£/kg (the green ammonia price in 2021). However, the H2-PEM has more potential on the lower end of hydrogen price, as shown in Fig. 16(a), (b).

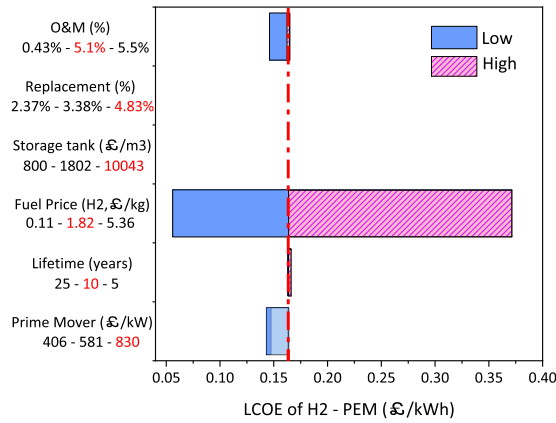


Fig. 16a. Sensitivity analysis of LCOE for H2-PEM based on low and high values for key model inputs.

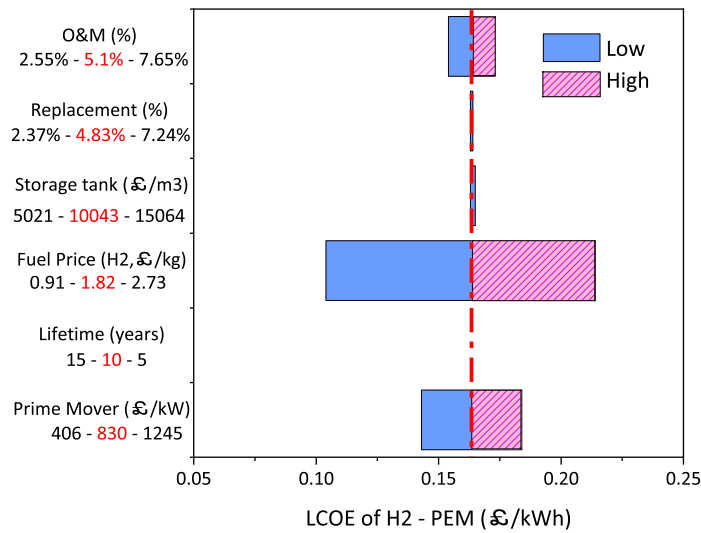


Fig. 16b. Sensitivity analysis of LCOE for H2-PEM based on low and high values for key model inputs with same change rate.

For NH3-SOFC, the prime mover price is the single most important variable as it directly affects the replacement (43% of prime mover price) and O&M (5.5% of prime mover price). International Energy Agency (IEA) also estimated that the CAPEX, O&M, and lifetime are the core influences for the SOFC to be a significant solution for transportation applications (IEA [Technology Collaboration Programme, 2019](#)). LCOE decreases by 76% if NH3-SOFC prime mover price decreases to 830£/kW, which has more economic advantage than and EMD-710 (0.143£/kWh) H2-PEM (0.164£/kWh). The SOFC could be more cost-effective if its CAPEX was to be lower than 1257/kW, which is forecasted to be the case by 2040 according to the IEA targets of SOFC (IEA [Technology Collaboration Programme, 2019](#)). Fig. 15 shows a moderate decrease in LCOE if the lifespan of NH3-SOFC improves from 10 years to 25 years. At 0.11£/kg ammonia price, decreasing or increasing the price of the storage tank has a small effect on the LCOE of NH3-SOFC.

For H2-PEM, LCOE is most sensitive to fuel cost and least sensitive to storage tank, lifespan, and replacement. It would have more advantages than ICE if the lower cost of fuel and PEMFCs could be achieved. Improving the PEM lifetime from 10 years to 25 years has a small effect on LCOE.

When the fuel cell power does not satisfy the need for traction such as the high traction force for startups or high speed, the batteries are discharged to meet the power demands. The battery cost is not considered in our economic case due to the train systems running smoothly on this route (Fig. 3), which results in small extra power needs from the batteries. To compensate for the demands of the complicated landscape in the UK and provide protection for fuel cells, four batteries (330 kWh, 440 kWh, 660 kWh, and 1275 kWh) are simulated in our dynamic models to analyse economic sensitivity. These simulations are based on previous works (Hoffrichter et al., 2016; Calvert et al., 2021; Zhang et al., 2022). The range of state of charge (SOC) is 20%-80%. According to the simulations, 330 kWh is the minimum battery capacity for powertrains.

The Li-ion batteries are considered in this research due to their advanced storage technologies for fuel cells and reliable lifespan. The CAPEX is around£277/kWh and O&M is 5.68% of CAPEX (National Renewable Energy Laboratory (NREL), 2021). The lifespan of

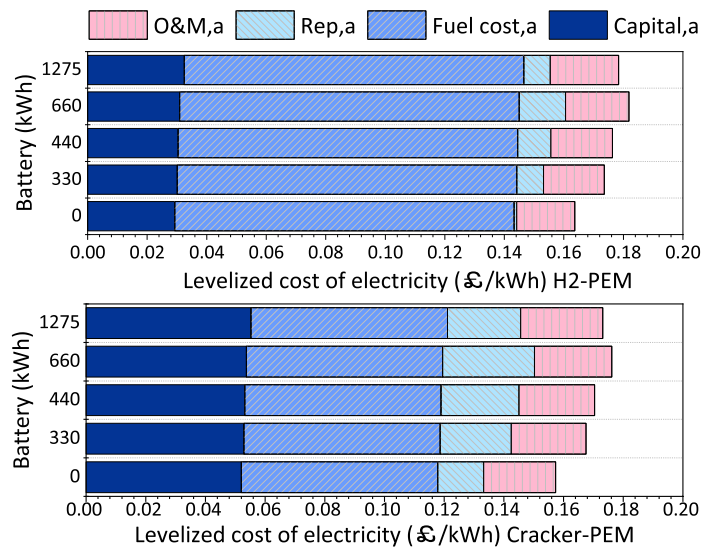


Fig. 17. The LCOE of H2-PEM and Cracker-PEM with batteries.

batteries is at the rated depth of discharge (Zakeri and Syri, 2015) (DoD) and 3000 full-depth charges (Zhang et al., 2022). The timescale of battery replacement can be deduced from their lifespans, the equation for which can be found in Eq (13).

For LCOE (Fig. 17), the replacement cost is 5%-9% higher than the case without batteries because the small-capacity batteries need more replacements than other facilities. The LCOE of cases with batteries is lower than that of EMD-710 (£0.332/kWh), NH3-SOFC (£0.542/kWh), and Cracker-SOFC (£0.347/kWh). As shown in Fig. 17, the cost of batteries has a relatively small impact on the economic evaluation of the different cases.

5. Conclusion

This study evaluated the potential application of ammonia as the fuel for a train running on a freight line from Felixstowe South Gbrf to Hams Hall Gbrf. The following performance metrics were considered: fuel cell powertrains efficiency, fuel consumption, fuel storage volume, and CO₂ emission. The metrics for economic evaluation were capital cost, operating and maintenance cost, replacement expenditure, fuel cost, Levelized cost of electricity, and discounted payback period.

The analysis of these metrics showed that ammonia has a feasible potential as fuel for freight rail. It provides a suitable link between diesel and hydrogen – it produces far fewer carbon emissions than diesel while needing less storage space and having safer fuel supply chain than hydrogen, making it ideal as a transition fuel from which hydrogen could be extracted. These advantages make ammonia a great alternative fuel for rail applications. Its versatility allows it to adapt to a variety of industrial requirements, making it a valuable transitional option for achieving decarbonisation goals.

Diesel trains are the most common type of train in the UK. It can be clearly seen from this study that EMD-710 is the most cost-effective solution scenario in LCOE (£0.144/kWh), benefitting from the high TRL and cheap cost. However, a clear disadvantage of diesel trains is their high level of carbon emissions per duty cycle. Hydrogen has long been identified as an alternative fuel that has the potential to replace fossil fuels. Its clear advantage is the lower carbon emissions when compared to diesel. However, while using PEM powertrains could achieve comparable LCOE (£0.164/kWh for H2-PEM, £0.157/kWh for Cracker-PEM) to diesel (£0.144/kWh), the high storage space required, expensive fuel and safety concerns limit its usability in current train applications. The volume of hydrogen tanks is thirteen times that of diesel tanks while the price of blue hydrogen is sixteen times the price of diesel. Additionally, for freight PEM trains, the lifespan of batteries is another challenge.

The volume of fuel storage can be decreased by switching from hydrogen to ammonia. Compared to hydrogen, ammonia storage tanks require 62% and 75% less space for Cracker-PEM and Cracker-SOFC, respectively. Cheap price is another advantage of brown ammonia. However, ammonia-fuelled cases face a stringent price range as opposed to the blue hydrogen and diesel-fuelled cases. When the ammonia price is cheaper than £0.4 /kg, the ammonia-fuelled Cracker PEM case makes more economic sense compared to the EMD-710 diesel engine using diesel at a price of £1.6 /kg. For the powertrains based on cracker, the efficiency of preheater and cracker have an influence on the fuel cost, which could also add to the cost of trains.

Direct ammonia-fuelled SOFC (NH₃-SOFC) drive systems could overcome these limits owing to SOFC best efficiency. Less storage space is needed for NH₃-SOFC compared to H2-PEM. Benefiting from the operating high temperature of SOFC, ammonia cracker and purifier are not required for NH₃-SOFC. However, the huge challenge with SOFCs is their low commercial readiness level as MW-scale SOFC and direct ammonia SOFC are still at the lab-level. SOFC powertrains might be viewed as a financially sound option if the overall cost of SOFC could be reduced by 70%.

This study shows the potential of ammonia as a fuel for freight trains in technical and economic terms. Currently, as per this study,

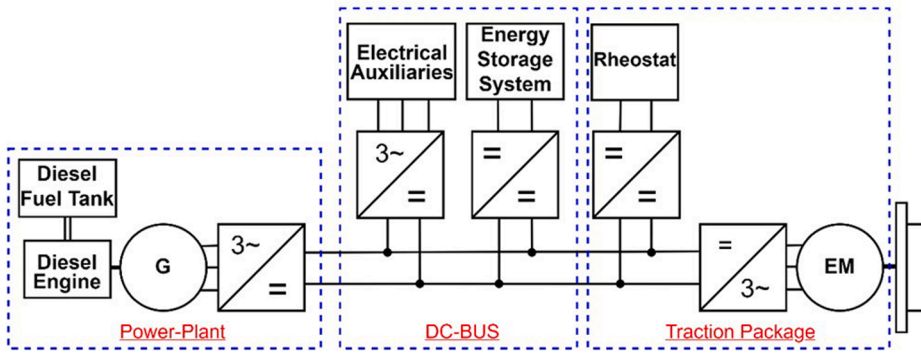


Fig. A1. Power-module drive-system diagrams of the diesel-electric locomotive.

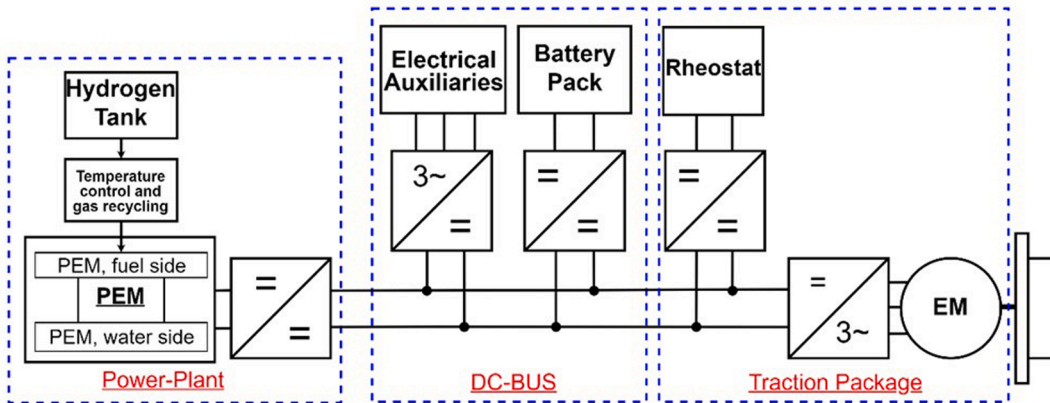


Fig. A2. Power-module drive-system diagrams of the H2-PEM locomotive.

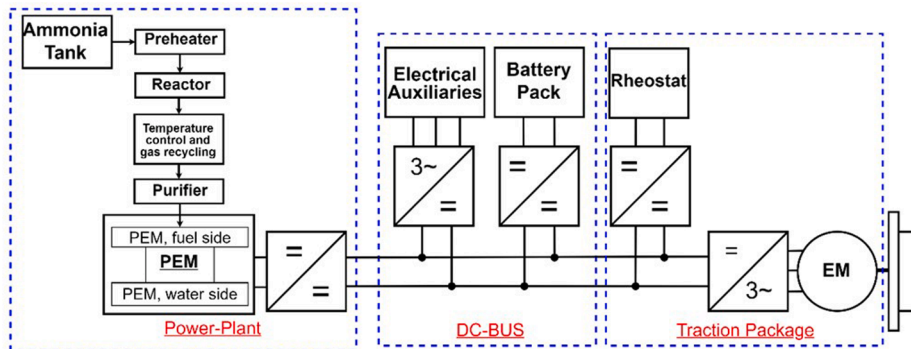


Fig. A3. Ammonia cracker-PEM powertrain configuration.

Ammonia-fuelled Cracker-PEM is the best option for train powertrains, when considering storage space and fuel cost, but the requirement for high technology of purifier poses a challenge. However, there is a possibility that this could change in the future. Ammonia-directed SOFC powertrain also shows great promise for freight trains, especially if its price is decreased while increasing its TRL. Further research and development of the ammonia-directed SOFC is required to discern whether it is possible to make this technology more cost-effective and able to deliver on higher power requirements.

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.

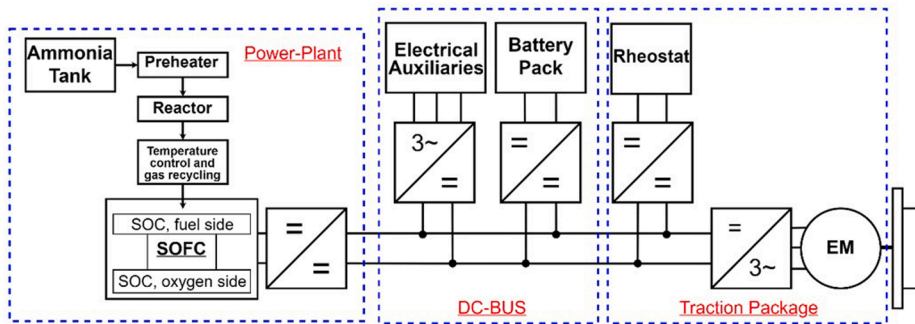


Fig. A4. Cracker-SOFC power system configuration.

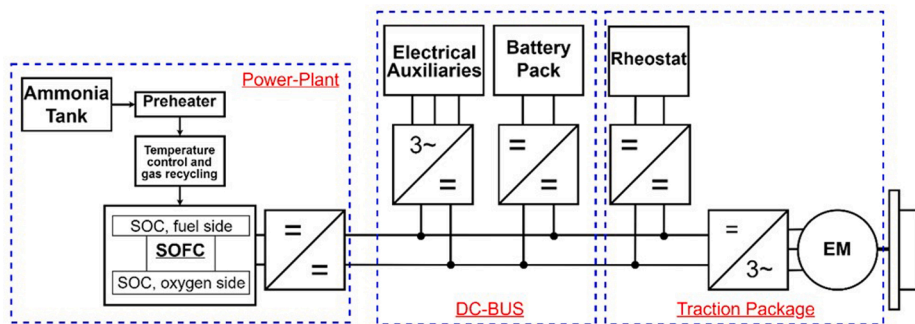


Fig. A5. Ammonia-fuelled SOFC power system configuration.

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Appendix

See Figs. A1-A5.

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