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Techno-economic analysis of large-scale green hydrogen production and storage

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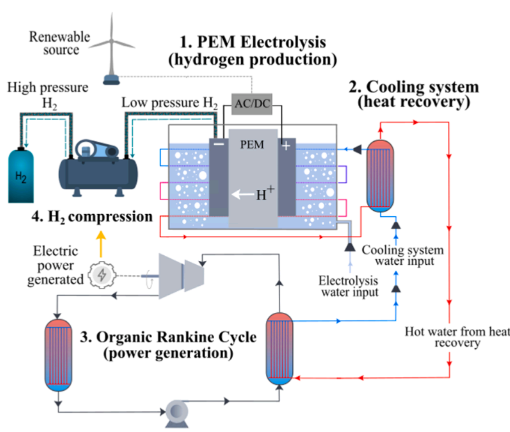
HIGHLIGHTS

- A 10-MW PEM electrolyser model with integrated heat recovery is presented.
- The model allows for simulating different PEM electrolysis plant sizes.
- Waste heat recovery increases overall efficiency from 71.4% to 98%.
- The feasibility of waste heat recovery with ORC is electricity price dependent.
- The load factor is a significant contributor to the LCOH.

GRAPHICAL ABSTRACT



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ABSTRACT

Producing clean energy and minimising energy waste are essential to achieve the United Nations sustainable development goals such as Sustainable Development Goal 7 and 13. This research analyses the techno-economic potential of waste heat recovery from multi-MW scale green hydrogen production. A 10 MW proton exchange membrane electrolysis process is modelled with a heat recovery system coupled with an organic Rankine cycle (ORC) to drive the mechanical compression of hydrogen. The technical results demonstrate that when implementing waste heat recovery coupled with an ORC, the first-law efficiency of electrolyser increases from 71.4% to 98%. The ORC can generate sufficient power to drive the hydrogen's compression from the outlet pressure at the electrolyser 30 bar, up to 200 bar. An economic analysis is conducted to calculate the levelised cost of hydrogen (LCOH) of system and assess the feasibility of implementing waste heat recovery coupled with ORC. The results reveal that electricity prices dominate the LCOH. When electricity prices are low (e.g., dedicated offshore wind electricity), the LCOH is higher when implementing heat recovery. The additional capital

Abbreviations: **AEL**, Alkaline Water Electrolysis; **CAPEX**, Capital Expenditure; **CCS**, Carbon Capture and Storage; **CCUS**, Carbon Capture, Utilisation and Storage; **GDP**, Gross domestic product; **GHG**, Greenhouse Gases; **GWP**, Global warming potential; **HHV**, Higher Heating Value; **LCOH**, Levelised Cost of Hydrogen; **LF**, Load Factor; **NPV**, Net Present Value; **OPEX**, Operating Expenditure; **ORC**, Organic Rankine Cycle; **PEM**, Proton Exchange Membrane; **SOEC**, Solid Oxide Electrolysis; **SMR**, Steam Methane Reforming; **SPE**, Solid Polymer Electrolyte.

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expenditure and operating expenditure associated with the ORC increases the LCOH and these additional costs outweigh the savings generated by not purchasing electricity for compression. On the other hand, heat recovery and ORC become attractive and feasible when grid electricity prices are higher.

1. Introduction

In order to tackle the current climate crisis and meet the Paris Agreement target of limiting the global temperature rise to 1.5 °C, different countries are taking urgent measures to decarbonise the most carbon-intensive sectors such as electricity and heat generation, transportation, and industry [1]. One of the preferred solutions to reduce global greenhouse gas (GHG) emissions from the energy sector are adopting renewable energy sources and displacing fossil fuels [2]. While the share of renewables continues to grow in the energy matrix, the intermittency challenge associated with these fluctuating energy sources needs to be solved. An alternative for using the excess energy from renewables is a Power-to-Gas approach by transforming or storing this extra energy into an energy carrier like hydrogen [3]. It is estimated that by 2030, there will be a potential to store in hydrogen up to 300TWh excess of electricity coming from solar and wind energy [1]. The sustainable pathways for energy transition identify hydrogen as an important vector of transition to enable renewable energy system integration at a large scale. Hydrogen presents storage capabilities for intermittent renewable electricity and has the potential to enhance the flexibility of the overall energy system [4]. Currently, the European Union and twelve more countries, which together sum up 44% of the global gross domestic product (GDP), have already established a national hydrogen strategy or roadmap [5]. The United Kingdom hydrogen strategy recognises the role of large-scale hydrogen as a lever to achieve the net-zero target by 2050 and the Sixth Carbon Budget (CB6), which aims to reduce emissions by 78% by 2035. Also, an ambitious target of 5 GW of low carbon hydrogen production capacity has been set for 2030 to enhance the country's hydrogen economy [6].

1.1. *Hydrogen production*

Hydrogen is not readily available in its pure elemental form on Earth, but there are different methods and energy sources to produce it. A colour system has been adopted to label hydrogen according to its production process and energy source. Grey hydrogen is produced by steam methane reforming (SMR) or coal gasification using fossil fuels as the energy source and emitting considerable CO_2 emissions during the process. Grey hydrogen can be converted into blue hydrogen by coupling it with carbon capture and storage (CCS) so that the hydrogen production process via this method becomes carbon neutral. Green hydrogen is produced using a renewable energy source to power the water electrolysis process resulting in a zero-carbon process [7]. Recently, other hydrogen colours have been added to the list, like pink hydrogen, which is water electrolysis using nuclear energy. Turquoise hydrogen consists in methane pyrolysis, which produces solid carbon rather than CO_2 [8].

Global hydrogen production currently relies almost on fossil fuels like natural gas and coal, reporting for 95% of the total amount produced and only 5% by electrolysis [7]. The global hydrogen demand in 2020 was estimated to be 90 Mt, from which 60% was created via SMR using natural gas. As fossil fuels are the primary source of hydrogen production, vast amounts of direct CO_2 emissions are linked. In 2020, hydrogen production accounted for 2.5% of global CO_2 emissions in the industry and energy sectors [9]. That is why methods to decarbonise hydrogen production, like carbon capture, utilisation, and storage (CCUS) and water electrolysis powered by renewable sources, are seen as a more promising way of hydrogen production in the near future. Moreover, the production process of hydrogen requires water. Contrary to what one might think, the electrolysis process requires less water (9 kg H_2O/kg H) than fossil fuel-based methods like natural gas with CCUS (13–18 kg H_2O/kg H) and coal gasification (40–85 kg H_2O/kg H) [9].

1.1.1. *Water electrolysis – Thermodynamics*

Water electrolysis to produce hydrogen can be achieved by three main methods: alkaline water electrolysis (AEL), solid oxide electrolysis (SOEC) and proton exchange membrane electrolysis (PEM). These electrolysis technologies differ according to the electrolyte separating the anode and the cathode, their materials, and their operating conditions.

Water electrolysis refers to the electrochemical process of production of hydrogen by applying a direct current electricity to water (H_2O) and separating it into hydrogen (H_2) at the cathode (hydrogen evolution reaction) and oxygen (O_2) at the anode (oxygen evolution reaction) as shown in the following equations:

Cathode:

$$2H^{+} + 2e^{-} \rightarrow H_2 \tag{1}$$

Anode:

$$H_2O \rightarrow \frac{1}{2}O_2 + 2H^{+} + 2e^{-} \tag{2}$$

Overall:

$$H_2O_l \rightarrow H_{2g} + \frac{1}{2}O_{2g} + Heat \tag{3}$$

1.1.2. *Proton exchange membrane (PEM) electrolyser*

A PEM electrolyser cell has a solid polymer electrolyte (SPE) separating the anode and the cathode. Fig. 1 contains a schematic of a PEM electrolyser cell showing that water (H_2O) is injected into the anode, where it reacts to form oxygen (O_2), positively charged hydrogen ions (protons) and electrons. The hydrogen ions (H^+) travel across the membrane to the cathode side. At the same time, the electrons in the anode flow through an external circuit to the cathode side to form the hydrogen (H_2) by recombining with the hydrogen ions [10,11].

PEM electrolysers have been recognised for having several advantages over other electrolysis technologies. Some of these advantages include a compact design, high current densities (>2 A/cm^2), high voltage efficiency, fast response to power input (in the order of millisecond), short start-up time, lower temperatures operation (50–80 °C), high gas purity of 99.99%, high operation pressure (approximately 80 bar) which results in the advantage of delivering hydrogen at a high output pressure hence requiring less energy for hydrogen compression and storage [10,12,13]. The response time of proton exchange

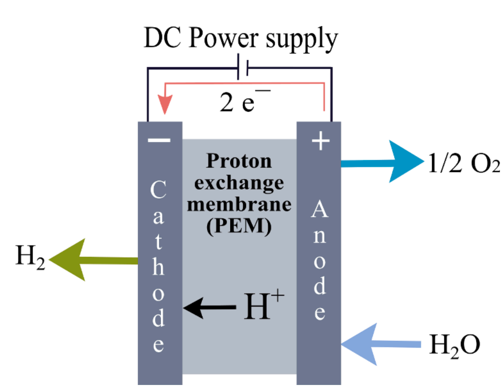

Fig. 1. Schematic of a PEM electrolyser cell.

membrane electrolyser is better than other electrolysis technologies, such as alkaline electrolysis. This is due to the unique properties of the PEM, which allow for rapid ion transport and efficient electrochemical reactions. PEM electrolysers can respond quickly to changes in the input power or hydrogen demand, which is essential for maintaining stable and efficient system operation. Additionally, PEM electrolysers operate at lower temperatures and pressures than other electrolysis technologies, which reduces the response time further. This faster response time allows the PEM electrolysers to be used in a wide range of applications, including renewable energy storage, hydrogen production, and fuel cell systems. The short start-up time and stable operation of PEM electrolysis represent a characteristic that makes this technology attractive to adequately react to the intermittent nature of renewable energies [14]. For example, Burrin et al. [11] proposed a novel combined heat and green hydrogen generator that utilised a PEM electrolysis system with heat recovery, resulting in improved hydrogen production rates and energy efficiency. Similarly, Zhang and Yuan [15] discussed the economic evaluation of hydrogen production by water electrolysis and examines the impact of power fluctuations on the efficiency and durability of proton exchange membrane electrolytic cells. The authors also discuss the economic feasibility of PEM electrolysis systems coupled with different wind power and photovoltaic power plants. The evaluation results indicate that the economics of PEM electrolysis systems, neither off-grid nor grid-connected, are unsatisfactory when evaluated with the available techno-economic parameters. The high efficiency and low operating costs, make them an attractive technology for a variety of industrial and commercial applications.

1.1.3. Hydrogen compression - auxiliary process of the hydrogen value chain

Amongst the non-nuclear fuels, hydrogen has the highest gravimetric energy density, which means that it has a high energy content per unit mass (Net caloric value = ~ 33 kWh/kg), making it an exceptional energy carrier. Nevertheless, the density of hydrogen (90 g/m^3) under atmospheric conditions is low compared to other gases [16]. This also means that hydrogen possesses a very low volumetric energy density (0.003 kWh/L), which is the amount of energy contained compared to its volume [17]. These characteristics represent various challenges in the hydrogen's value chain, going from storage, distribution/transportation, and utilisation. If maintained at atmospheric conditions, hydrogen gas would require a considerable amount of space to be stored; hence its density needs to be increased. Compression has proven to be the most straightforward and a very effective technique to increase hydrogen density and storage capacity. That is why, at the moment, storing hydrogen as a compressed gas in metal cylinders at various pressures is the most used method [18].

Moreover, new, and emerging technologies require the utilisation of hydrogen at high pressures to satisfy diverse process requirements for different hydrogen applications. For use in industry or laboratories, hydrogen is commonly compressed to 150–200 bar pressures. Fuel cell vehicles use hydrogen that has been pressurised to 350–700 bar and kept in onboard storage tanks. Gaseous hydrogen is pressurised in stages (up to 100 bar) at hydrogen refuelling stations before being stored in banks of containers. For instance, a refuelling station with gaseous hydrogen storage can employ three distinct pressure levels: low-pressure storage in cigar tanks (45 bar), medium-pressure storage in a group of cylinders (200–500 bar), and high-pressure storage in composite cylinders (700–1000 bar) [19].

Mechanical compressors are the most used hydrogen compression technology nowadays. The technology behind mechanical hydrogen compressors is quite advanced and mature. However, the amount of energy required for hydrogen compression is one of its main concerns because it rises as the outlet pressure increases [17].

1.1.4. Waste heat recovery – Organic Rankine cycle (ORC)

The energy efficiency of PEM electrolysers is expected to be in the range of 70% [11], as the remaining energy is translated into waste heat. With the growing interest in green hydrogen, attention has been focused on the amount of hydrogen generated through water electrolysis. Not much attention has been given to the waste heat vented to the surroundings. Moreover, recovering the waste heat could increase overall efficiency of the system. With the deployment of large-scale electrolysers, there is a huge opportunity to take advantage of waste heat in the order of MW, as it becomes more viable and cost-effective to recover and use.

A preferred method for waste heat recovery is the creation of electrical power, which may employ thermal energy in various low-temperature cycles. The organic Rankine cycle is a proven method for effectively converting low and medium-temperature heat sources, in the range of 50–300 °C, into electricity and has long been recognised as a viable approach to recovering waste heat [20,21]. As depicted in Fig. 2, four elements comprise a basic ORC: a pump, an evaporator, an expansion device (generally a turbine), and a condenser. An organic working fluid is heated in a boiler until it is converted to vapour; then, it flows through a turbine where it is expanded, producing work (which can be converted into electricity if coupled to a generator). After the turbine, the gas is then condensed, and the cycle is repeated by passing the condensed fluid through a pump, which raises the fluid's pressure, making it ready to enter the boiler again [21]. The working fluid is continually circulated through the four components of this closed-loop system to transform thermal energy into mechanical/electrical power. ORC systems have been studied and analysed in many studies. Peris et al. [22] described an experimental application of an ORC in a ceramic industry for low-grade waste heat recovery. The study aimed to verify the ORC's performance in actual industrial conditions. The ORC's performance was experimentally characterized in a test bench, achieving a maximum gross electrical efficiency of 12.32%. Kim et al. [23] evaluated the performance of a small-scale ORC system that uses low-grade heat at a temperature below 80 °C and has a cycle power of less than 10 kW. The study established a performance map for investigating optimal operating conditions, which revealed that the net power and efficiency of the system increased with increasing heat source temperature, making such systems feasible for productive utilisation of waste heat, and reducing thermal pollution. In another study, Veloso et al. [24] discussed the application of ORC for power generation in a Brazilian FPSO platform. They evaluated the thermodynamic performance of the ORC cycle using a computational tool developed in MATLAB. The study finds that the application of ORC cycles on FPSO platforms for heat recovery from low-temperature sources allows for an essential increase in energy and exergetic efficiency and contributes to a significant reduction in greenhouse gas emissions. Salari and Hakkaki-Fard [25] evaluated the performance of a photovoltaic thermal ORC system combined

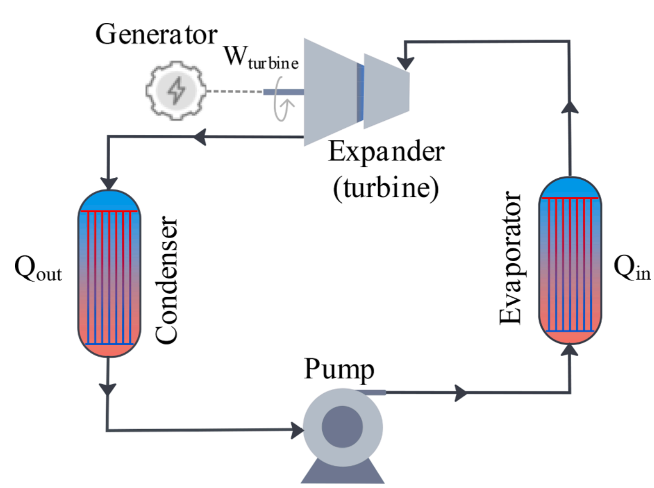

Fig. 2. Schematic of a basic ORC.

with a PEM electrolysis cell. A combined numerical/theoretical model is used to evaluate the system's performance with different working fluids and operating conditions. Results show that the proposed integrated system has a higher electrical efficiency than conventional photovoltaic thermal systems and can produce a maximum hydrogen production rate of 1.70 mol/h.

1.2. Aim and novelty

Building on the above ideas, this study analyses the techno-economic potential of waste heat recovery from multi-MW scale green hydrogen production process. The novelty of this study falls on modelling a 10-MW electrolysis system with its respective hydrogen compression. The study analyses the potential of using the waste heat, which is typically exhausted into the environment, in an ORC to produce the electricity needed to power the compression process of hydrogen.

2. Methodology

The software Aspen Plus® is used for the modelling and the simulation of the 10 MW PEM electrolysis process with a cooling system used for heat recovery and coupled with an ORC to power the mechanical compression of hydrogen.

2.1. Technical analysis

The electrolyser model is built and adapted to analyse three different case scenarios in which the output hydrogen gas stream is given at different pressures after compression: 200 bar, 350 bar and 700 bar. The objective of the technical analysis is to investigate the quality and quantity of the recoverable waste heat available from the electrolysis process and to determine the amount of power needed for compressing the hydrogen at the three desired pressures. Each flowsheet for these three cases aims to validate the technical feasibility of utilising the excess thermal energy to drive an ORC to generate electricity. For each scenario, it is analysed if the generated power from the ORC is sufficient to drive the hydrogen mechanical compression process and the additional electrical requirement when the power is found to be insufficient.

2.2. Economic analysis

The economic evaluation for this study uses the levelised cost of hydrogen (LCOH) approach to assess the cost of the 10-MW PEM electrolysis plant, including capital expenditure (CAPEX), variable and fixed operating expenditures (OPEX), and electricity costs. The economic analysis (Section 5) compares the LCOH of the model before and after implementing the waste heat recovery to evaluate its feasibility. Moreover, it describes three different scenarios of hydrogen compression, load factors and electricity costs to demonstrate a variety of representative LCOH estimations for the system.

3. PEM Electrolyser Model Development

As shown in Fig. 3, the integrated PEM electrolysis system includes the hydrogen production by a 10-MW PEM electrolysis process, the hydrogen compression process, the cooling system to capture the waste heat, and the ORC system to produce the power needed for hydrogen compression. A visual representation of the Aspen model flowsheets refers to Fig. 4.

Traditionally, PEM electrolysis systems have been developed on a small scale. To achieve large-scale electrolysis plants in the multi-MW range, the current practice is to connect in parallel as many electrolysers as necessary, in the range from 1 to 2 MW, until the required size is obtained [12,26]. Manufacturers like ITM power and H-TEC Systems offer standardised PEM electrolysers modules that can be aggregated to enable a higher range of capacities [27–29]. Following this principle, to reach the 10-MW PEM electrolyser simulation in Aspen, the first step is to develop a standardised model of a 2-MW PEM electrolyser and then group five of them together to get the desired capacity of 10 MW.

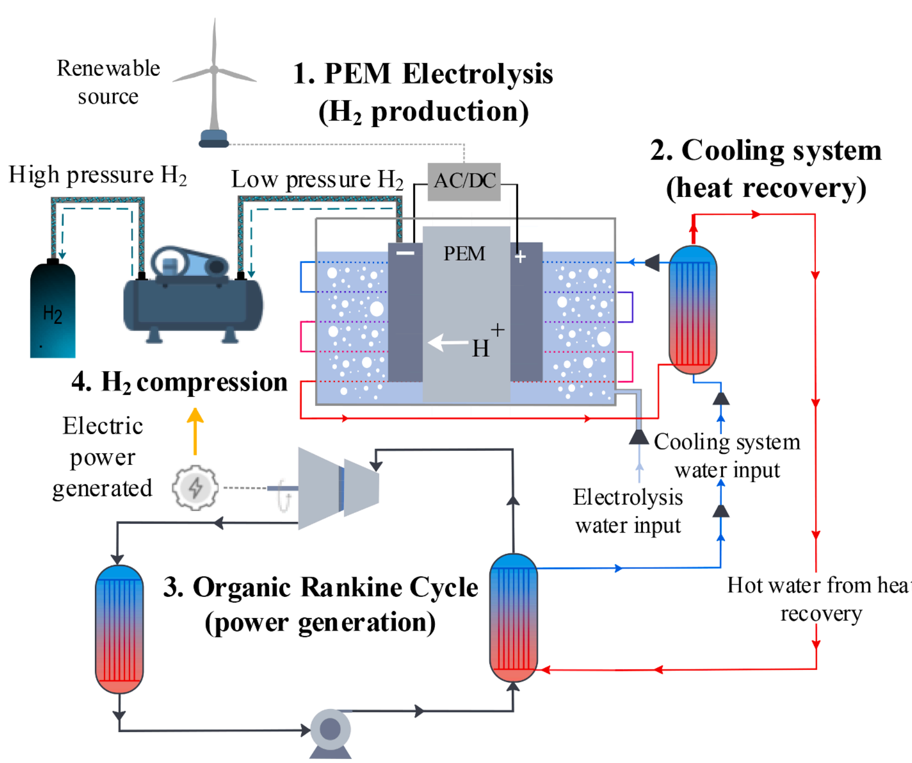

Fig. 3. Schematic of integrated PEM electrolysis system with heat recovery for hydrogen compression.

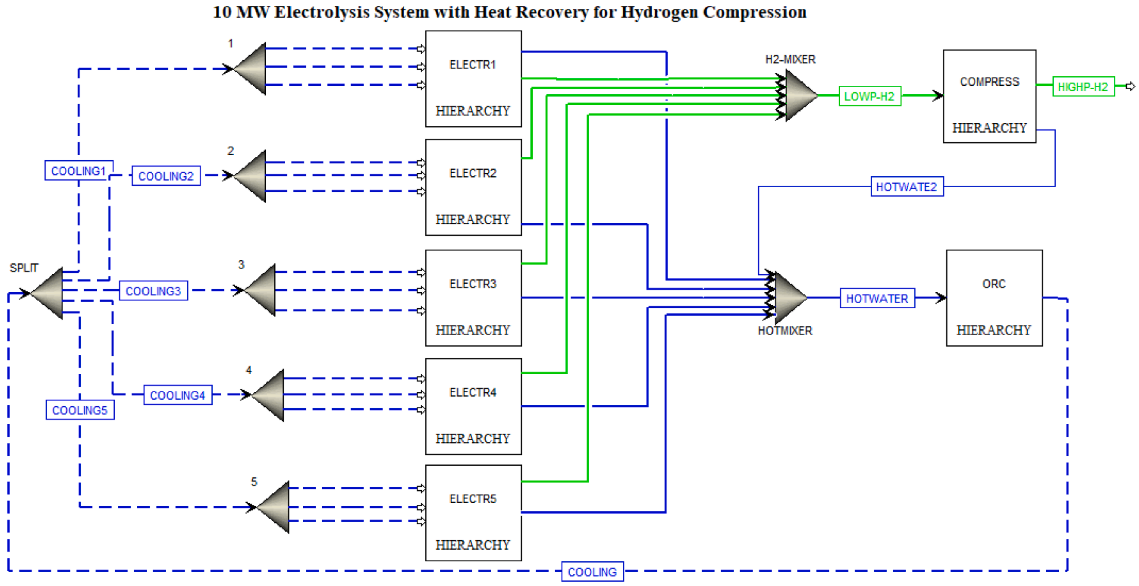

Fig. 4. Schematic of full Aspen Plus® model integration for a 10-MW PEM electrolysis plant.

3.1. Standardised 2 MW PEM electrolyser with heat recovery

The 2 MW PEM electrolyser model shown in Fig. 5 was developed, tuned and validated by taking into account operational and design parameters from industry leading manufacturers [29,30] and relevant literatures [11,12,26]. Table 1 presents the operating parameters of the proposed 2 MW-scale PEM electrolyser model.

The PEM stack is fed with two streams. The first stream is an input of 2 MW of electricity from a renewable energy source. The second stream is deionised water at ambient temperature and pressure (20 °C and 1 bar). The operating conditions of PEM stack are defined as a temperature of 80 °C and a pressure of 30 bar. Inside the PEM stack, the model simulates the electrolysis process shown on Equations 1–3, where the water split reaction occurs, and water is transformed into hydrogen and oxygen. The hydrogen and oxygen gas mixture are then separated between the cathode and anode sections, respectively. It is known that

Table 1
Operating parameters of the 2-MW PEM electrolyser with integrated cooling system for heat recovery.

System	Parameters	Values
2 MW PEM Electrolyser	Power input (kW)	2,000
	Electrolysis water input (kg/h)	324
	Hydrogen production (kg/h)	36.26
	Hydrogen output pressure (bar)	30
	Hydrogen production power-equivalent (kW)	1,428.6
	Oxygen production (kg/h)	287.74
Cooling system	Water mass flow (kg/h)	14,160
	Water outlet temperature (°C)	76
	Heat extracted in cooling circuit (kW)	565

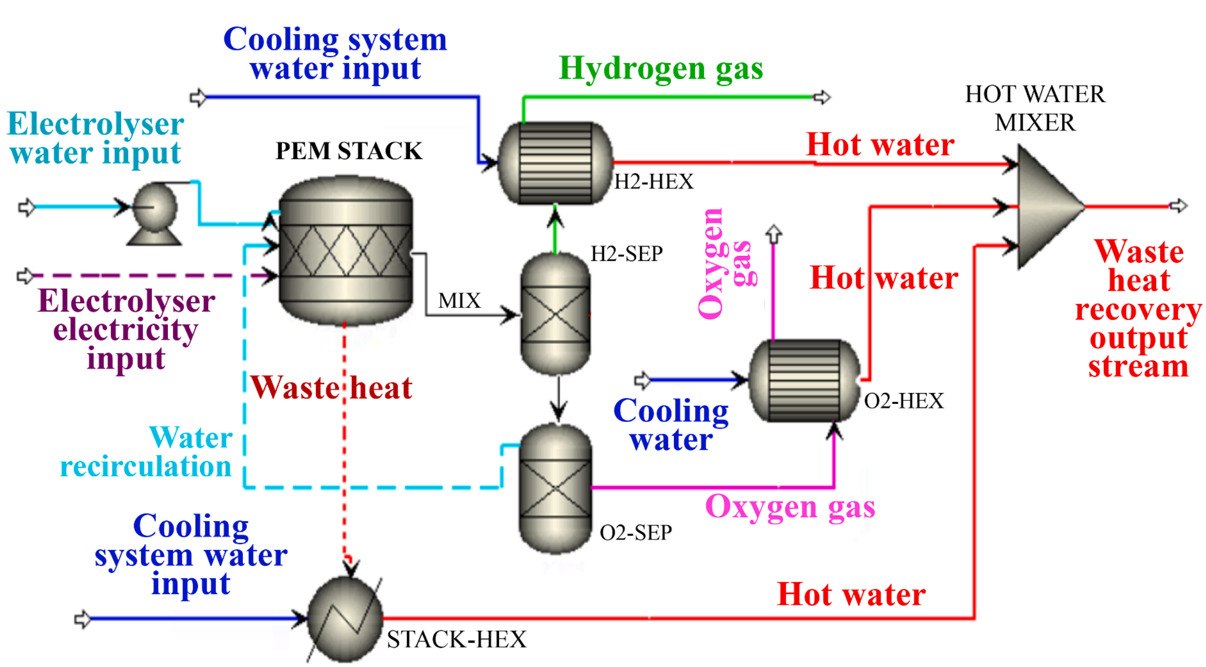

Fig. 5. Model of a 2 MW PEM electrolyser with integrated cooling system for heat recovery.

PEM electrolysers do not have a 100% reaction rate; hence the unreacted water is recirculated into the stack to avoid loss of heated water.

Currently, most auxiliary cooling systems of electrolyser are designed to keep the stack within the desired temperature range, removing the excess heat and venting it into the environment. However, since this research aims to analyse the potential of using the waste thermal energy, the cooling system is designed to extract available waste heat and reutilise it in the subsequent step of the process, which is hydrogen compression. As shown in Fig. 5, the cooling system comprises a set of heat exchangers (STACK-HEX, H_2-HEX and O_2-HEX) capable of capturing the thermal energy from the PEM stack and the gas streams of hydrogen and oxygen.

To cool down the stack and capture this amount of thermal energy, cooling water at 20 °C and 1 bar extracts the heat, resulting in an outlet flow of hot water. The thermal energy contained in each gas stream is captured separately by an individual heat exchanger designed for each stream. Inside each heat exchanger, heat is removed from the hot gas by a stream of cooling water at 20 °C and 1 bar. The three output streams from the cooling system are mixed together, which formed a single hot water output stream with a mass flow of 14,160 kg/h at a temperature of 76 °C.

3.1.1. Model characterisation

In this section, we evaluate the performance of our 2 MW PEM electrolyser model and compare it with the existing PEM electrolyser technologies offered in the market by leading manufacturers. We focus on two representative products: the 3 MEP Cube from ITM Power and the Hydrogen Cube System (HCS) from H-TEC Systems. Both products are modular and containerised for large-scale PEM electrolysis applications.

The 3 MEP Cube is a 2 MW PEM electrolyser that can produce up to 36 kg/h of hydrogen at an output pressure of 30 bar with a stack efficiency of 75% and a system efficiency of 65% at nominal power [31]. The Hydrogen Cube System (HCS) is another 2 MW PEM electrolyser that can produce up to 37.5 kg/h of hydrogen at an output pressure ranging from 15 to 30 bar and it has a stack efficiency of 80% and a system efficiency of 70% at nominal power [28].

Table 2 summarises the main operating parameters and efficiencies of our model and the two products. The electrolyser model was also used and validated in our previous work for a 1 MW system [11]. As can be seen, our model achieves comparable results with the current state-of-the-art PEM technology in terms of hydrogen production, output pressure, stack efficiency and system efficiency.

3.2. 10 MW PEM electrolyser system

Once the 2 MW PEM electrolyser system has been tuned and validated, the next step is to aggregate five of these standardised models to reach a 10 MW electrolyser capacity. The individual relevant flows of each electrolyser, such as hydrogen gas stream and hot water, are grouped into the same streams to analyse the system in an integrated way. The operating parameters are shown in Table 3. Hydrogen gas outputs are channelled into a single stream with a flow rate of 181.3 kg/h at 30 bar and 25 °C. Similarly, the hot water streams coming from the heat recovery systems are combined into a single flow of 70,800 kg/h at 76 °C.

Table 2
Comparison between proposed 2-MW scale system and existing PEM electrolyser technologies.

	Proposed model	3 MEP Cube (ITM)	HCS (H-TEC)
Electric power input (MW)	2	2	2
Hydrogen production (kg/h)	36.26	36	37.5
Output pressure (bar)	30	30	15–30

Table 3
Operating parameters of the 10 MW PEM electrolyser with integrated cooling system for heat recovery.

System	Parameters	Values
10 MW PEM Electrolyser	Power input (kW)	10,000
	Electrolysis water input (kg/h)	1,620
	Hydrogen production (kg/h)	181.3
	Hydrogen output pressure (bar)	30
	Hydrogen production power-equivalent (kW)	7,143.2
	Oxygen production (kg/h)	1,438.7
Cooling system	Water mass flow (kg/h)	70,800
	Water outlet temperature (°C)	76
	Heat extracted in cooling circuit (kW)	2,827

3.3. Hydrogen compression

The desired output of this PEM electrolysis plant is high-pressure hydrogen. Hence, the hydrogen output stream is compressed using a multi-stage mechanical compression process. As explained previously, different output pressures of hydrogen are required to achieve the necessary conditions for storage, transportation, and utilisation. Also, high pressurised hydrogen is needed to meet diverse processes requirements and new technologies for hydrogen applications. Consequently, the simulation model was designed to compress hydrogen from 30 bar, which is the output pressure at the electrolysers, up to 200 bar, 350 bar and 700 bar. These three scenarios represent the most required high-pressure hydrogen outputs.

The hydrogen compression process is simulated using a multi-stage compression unit operator, which sets up limit conditions for the temperature rise of the gas and the pressure output at each stage. The conditions are specified for the three desired hydrogen output pressure scenarios. The hydrogen compression process also entails a quantity of rejected waste heat, for which a heat recovery system is included for each compression scenario. The heat recovery system consists of a heat exchanger that recovers the waste thermal energy through a flow of cold water at ambient conditions (20 °C and 1 bar). The outlet stream contains hot water at a temperature equal to that coming from heat recovery system of the electrolysers (76 °C) to feed them together to the ORC. Fig. 6 presents the multi-stage hydrogen compression model for the compression scenario of 350 bar, with its respective heat recovery system. The compressor performance is simulated using Aspen Plus®, and the results were analysed to determine the efficiency, power consumption, and outlet gas conditions. The compressor stages were optimised to achieve the desired compression ratio from 30 bar to 350 bar, and the system design and operating conditions were adjusted accordingly. Each stage of compression process includes a compressor, an inter-cooler, and a flash. Inter-cooler is used for condensation of water and flash is used to separate hydrogen gas stream and condensed water.

3.4. Heat recovery system integration and organic Rankine cycle (ORC)

The heat recovery systems from the 10 MW PEM electrolysis process and from the hydrogen compression are configured which has output water temperature of 76 °C, having a suitable temperature for the ORC. The output streams are mixed to form a single hot water stream that will be used as the heat transfer fluid in the ORC boiler/evaporator. The selection of a working fluid is one of the crucial steps in the design of an ORC system, as it can significantly affect its performance and efficiency. Various studies on working fluids for ORC show that the refrigerant R245fa is a convenient fluid for recovering low-temperature heat sources as it has a boiling point of 15.3 °C [20,32,33]. Additionally, R245fa has a low viscosity, which reduces the pumping power required in the ORC system and R245fa is commercially available and widely used in

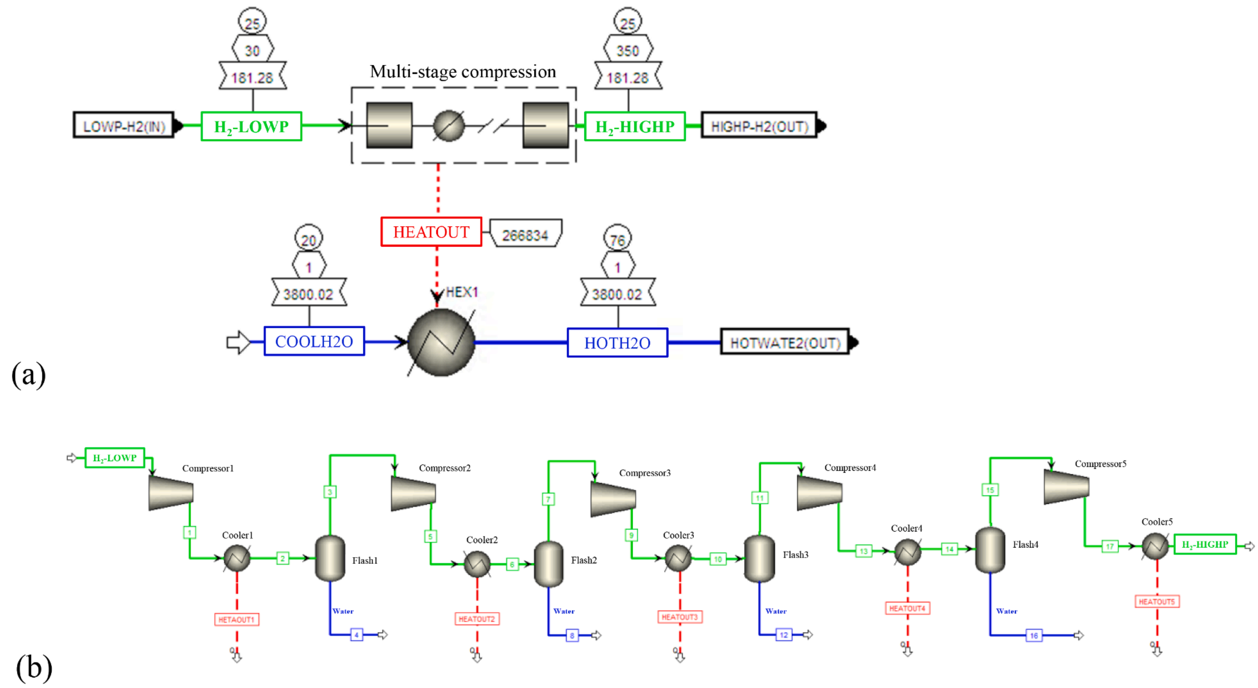

Fig. 6. Model of the multi-stage hydrogen compression to 350 bars with heat recovery system: (a) overall process; (b) multi-stage compression process.

the refrigeration and air conditioning industry. Several alternative working fluids are available for ORC systems, each of these working fluids has their advantages and disadvantages. For instance, R123 has a lower global warming potential (GWP) than R245fa but has a higher toxicity and flammability. Isobutane has a lower GWP than R245fa, but its flammability limits its use in some applications.

Based on this criterion, R245fa is selected as the working fluid for modelling the process. According to the three hydrogen compression scenarios (200 bar, 350 bar and 700 bar), different ORC models are designed and simulated to analyse the amount of power generated by the ORC and compare it against the energy needed for compression.

Fig. 7 shows the ORC model for the 350-bar compression scenario and their input parameters are listed in Table 4. The ORC model has been built and validated in our previous study [32]. A stream of hot water at 76 °C, coming from the heat recovery system, enters the evaporator (EVA) and transfers its heat to the R245fa working fluid. This heat exchange produces a rise in the temperature of the fluid, causing its

Table 4
Input parameters of the ORC model for the 350-bar scenario in Aspen Plus.

Section	Parameter	Value
Fluid pump	Discharge pressure	2.45 bar
	Efficiency	0.7
Evaporator	Cold stream outlet vapour fraction	1
Expander	Discharge pressure	1.0076 bar
	Isentropic efficiency	0.7
Condenser	Hot stream outlet vapor fraction	0
Working fluid	Mass flow rate	87,000 kg/h
Hot stream	Mass flow rate	74,600 kg/h
	Inlet temperature	76 °C
Cold stream	Mass flow rate	790,000 kg/h
	Cooling temperature	15 °C

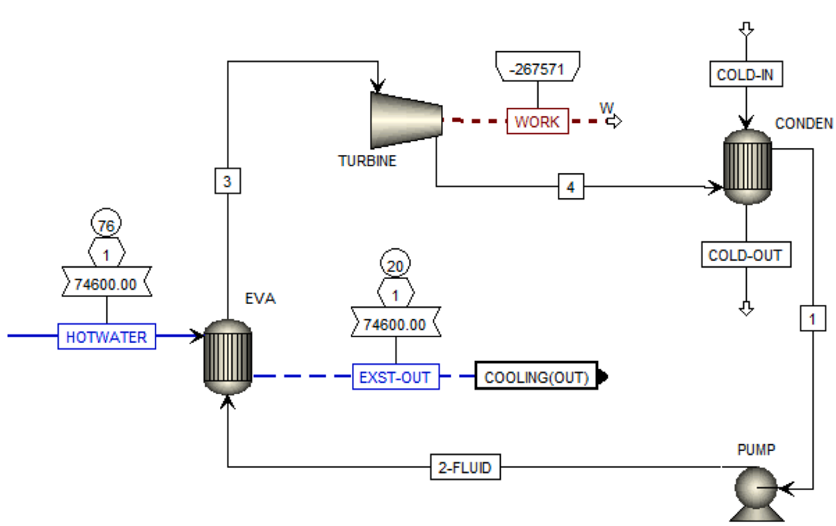

Fig. 7. Model of the Organic Rankine Cycle for the 350-bar compression scenario.

phase to change into a vapour. A superheated temperature of 5 °C is assumed for working fluid after its evaporation. After the heat exchange happens, the water leaves the evaporator at 20 °C, ready to be pumped back into the electrolysis cooling system (heat recovery system). The vaporised fluid then passes through the turbine. Here, the vapour expands, producing the turbine to spin and generate work. After going through the turbine, the vaporised organic fluid is cooled and converted back to a liquid in the condenser. The cycle repeats when a pump pressurises the liquid and drives it into the evaporator. The turbine is coupled with a generator to produces the necessary electricity to power the compression process of hydrogen.

The total efficiency of the ORC system η_{system} can be calculated by the difference between the work of turbine $W_{turbine}$ and pump work W_{pump}, divided by the transferred heat Q_{in} into the system, as shown in Equation (4) [33].

$$\eta_{system} = \frac{W_{turbine} - W_{pump}}{Q_{in}} \tag{4}$$

4. Results and discussion: technical analysis

4.1. Hydrogen production and heat recovery in 10 MW PEM electrolyser

The 10 MW PEM electrolyser model produces 181.3 kg of hydrogen per hour. Based on the higher heating value (HHV) of hydrogen, this hydrogen production represents an equivalent of 7,143 kWh (H_2 HHV = 39.4 kWh/kg). For each 10 MW of input electricity into the electrolyser, 2,827 kW are lost as excess heat coming from the five PEM stacks and the hydrogen and oxygen gas streams. This means that an equivalent to 28.2% of the power input is available and recoverable as thermal energy.

The five PEM stacks that collectively reject 2,765 kW of thermal energy are responsible for the bulk of the available and recoverable heat from the electrolyser. As a consequence of the high temperature operating condition of the PEM stack, after the electrolysis process, the output hydrogen and oxygen gases are ejected at a temperature of 80 °C. The streams of these gases account for 62 kW of the recoverable waste heat. As a result, the integrated heat recovery system from the 10 MW PEM model (five electrolysers) can capture 2,827 kW of all the excess heat produced.

Fig. 8 presents the energy flow within the system and demonstrates that most of the system output is made up of energy that is present in the hydrogen gas itself. Therefore, the electrical conversion efficiency of system is 71.4%. As previously explained, some waste heat may be recovered and used to create electrical power. Even though some waste heat must ultimately be rejected into the environment, the total thermal efficiency of the system will be improved by recuperating this available heat from the PEM stacks and gas streams. The reutilisation of this thermal energy will enhance the system efficiency, reaching 98% efficiency.

4.2. Hydrogen compression scenarios and power produced by the ORC

The models for each hydrogen compression scenario generate the necessary information about the excess waste heat that is accessible, showing the corresponding output streams and mass flow to perform the compression. As shown in Fig. 9, the required amount of energy for hydrogen compression raises with respect to the desired outlet hydrogen gas pressure. If we analyse the percentage of equivalent energy of the produced hydrogen in comparison with the energy required for its compression, it could be translated into a fraction of its own energy that is being lost when it is compressed at certain high pressures. Therefore, when hydrogen is compressed at 200 bar, 350 bar, and 700 bar, the percentages of lost hydrogen equivalent energy are 3%, 4%, and 5%, respectively. Moreover, the total power produced by the ORC system for the three hydrogen compression scenarios also increases with higher outlet pressure requirements, as explained in the following subsections.

4.2.1. Scenario 1: 200 bar

The first scenario shows that for compressing hydrogen from 30 bar, which is its outlet pressure at the electrolyser, up to 200 bar, a total of

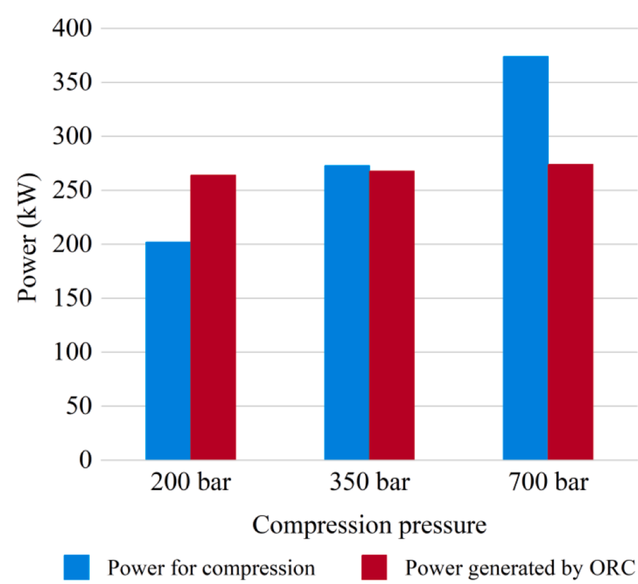

Fig. 9. Organic Rankine Cycle (ORC) power generation comparison for different hydrogen compression scenarios.

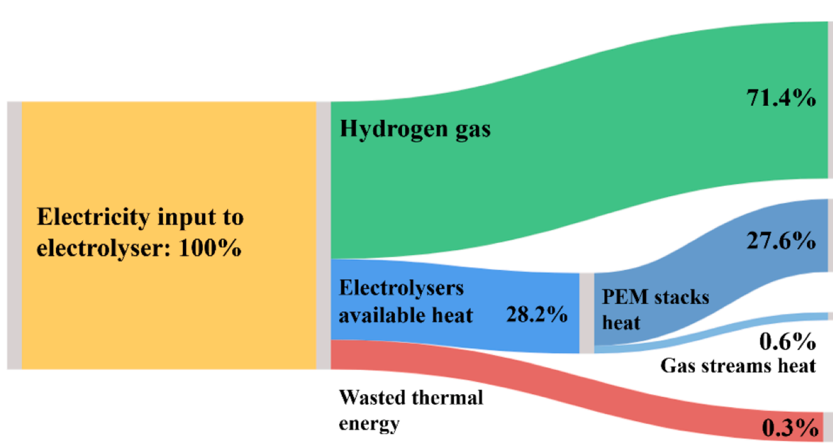

Fig. 8. Sankey diagram of energy flow within the electrolysis process.

202 kW electricity is needed. The ORC for this scenario can produce 264 kW electricity, which completely covers the power requirement for hydrogen compression, and even 62 kW remain unused. This remaining 62 kW electricity can be fed into the PEM stack for the electrolysis process.

4.2.2. Scenario 2: 350 bar

The second scenario, in which hydrogen is compressed to 350 bar, needs 273 kW electricity for hydrogen compression. The ORC for this scenario can produce 268 kW electricity, revealing that the ORC covers 98% of the power requirement for the compression. However, additional 6 kW electricity are needed to complete full hydrogen compression, accounting to 2% of power needed for hydrogen compression.

4.2.3. Scenario 3: 700 bar

Finally, hydrogen needs to be compressed from 30 bar to 700 bar in the third scenario, which requires 374 kW electricity supply. The ORC cannot completely fulfil the power requirements since it can only generate 274 kW power from recovered heat. The compression process requires an additional amount of 100 kW, which represents 27% of extra energy that needs to come from another power source different from the ORC.

4.2.4. ORC system efficiency

Various factors affect the thermal efficiency of an ORC. To mention the most relevant ones, we must consider the operational parameters of heat source, the thermodynamic properties of working fluid, and the system configuration. The thermal efficiency of an ORC system typically ranges between 2% and 19% on average, with lower thermal efficiencies in the range of 5 to 10% for smaller basic ORC systems [21,33]. Using Equation (4), the efficiency of the ORC model is calculated to be around 8%, which is in line with the current literature review findings. Fig. 10 presents energy flow of the integrated system combining the electrolysis process, the ORC, and the compression process for 350 bar hydrogen. Final compressed hydrogen product accounts for 69.5% of energy input, while 0.35% of the input electricity cannot be recovered. Around 92% of energy input to the ORC ends up wasted in the form of cooling water. It can be found that the electricity generated from ORC to the compression, and the recovered heat from compression to the ORC essentially become a closed loop.

4.3. Integrated heat recovery system

As shown in Table 5, the amount of recovered waste heat increases with a higher outlet pressure of hydrogen gas. This is mainly because with an increasing hydrogen outlet pressure, the compression process rejects more waste heat. Hence, there is more available thermal energy to be recovered.

5. Economic Analysis

5.1. Levelised cost of hydrogen (LCOH)

The levelised cost of hydrogen LCOH, given as a cost per energy unit of hydrogen generated (£/MWh H_2 HHV) or as a cost per mass unit of produced hydrogen (£/kg), is the discounted lifetime cost of constructing and running a facility of hydrogen production. It includes all pertinent expenses incurred during the lifespan of system, such as CAPEX, OPEX and electricity costs.

The LCOH approach is used to assess the economic feasibility of implementing waste heat recovery for powering the hydrogen compression process on the 10 MW PEM electrolysis system. The selected hydrogen compression scenario for the analysis is the 200-bar output pressure, in which the ORC system can completely cover the compression electric requirement. The economic analysis is conducted by first calculating the LCOH of the system without heat recovery and then calculating the LCOH of the system once waste heat recovery is implemented.

Equations 5–7 show how the LCOH was estimated using the net

Table 5
Heat recovery analysis for different hydrogen outlet pressure scenarios.

Hydrogen outlet pressure (bar)	30	200	350	700
Total power input (kW)*	10,000	10,202	10,273	10,374
Recovered waste heat from electrolysis process (kW)	2,827	2,827	2,827	2,827
Recovered waste heat from compression (kW)	\	199	267	358
Total recovered waste heat (%)*	28.2	29.7	30.1	30.7

[*] The total amounts for the hydrogen compression scenarios (200 bar, 350 bar and 700 bar) include both the electrolysis and compression processes.

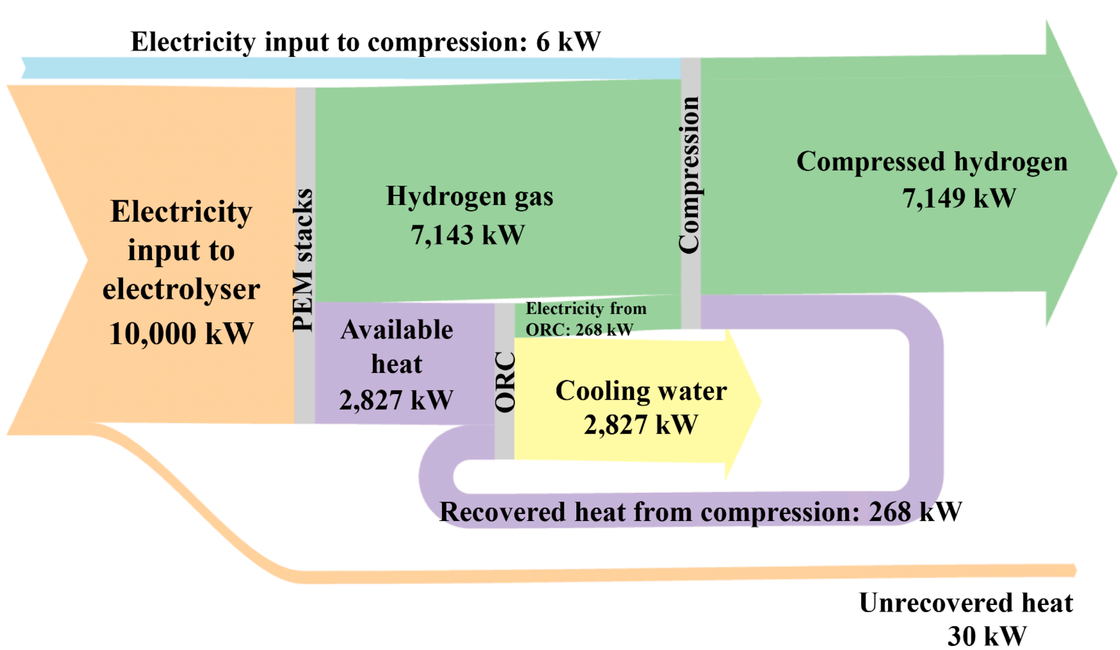

Fig. 10. Energy flow of the integrated electrolysis-ORC-compression system for 350-bar compression scenario.

present value (NPV) of the total costs and the NPV of the hydrogen production.

$$TotalCostsNPV = \sum_{n}^{N} \frac{C_n}{(1+d)^n} \quad (5)$$

$$HydrogenNPV = \sum_{n}^{N} \frac{Q_n}{(1+d)^n} \quad (6)$$

$$LCOH = \frac{TotalCostsNPV}{HydrogenNPV} \quad (7)$$

where N is the system's operating lifetime in years; n is the evaluated year; d is the discount rate; C_n is the cost in period n (including CAPEX, OPEX and electricity costs); and Q_n is the hydrogen production in period n. CAPEX is calculated using the total initial investment C_{inv} and the total replacement costs over the lifetime $C_{repl,t}$ as denoted in the equation below [34]. The cost of electricity C_{elec} consumed for hydrogen production is calculated as Equation (9).

$$CAPEX = C_{inv} + C_{repl,t} \quad (8)$$

$$C_{elec} = Price_{elec} \times E_{in,H_2} \times h \quad (9)$$

where $Price_{elec}$ is the market price for electricity, E_{in,H_2} is total electricity input for hydrogen production, and h is the operating hours which is determined by the load factor of electricity.

The Hydrogen Production Costs 2021 report [35] and the Hydrogen Supply Chain Evidence report [36], are consulted to obtain the official and most recent data for 10 MW PEM electrolysis plants. The data matches the plant size of the PEM electrolysis modelled in this study; hence, the CAPEX and OPEX costs are mainly gathered from those sources. The results obtained from the model are used to calculate the annual production of hydrogen. The extended list of the technical and cost assumptions used for the LCOH calculations can be consulted in Table 6.

5.1.1. Load factors and electricity prices

The LCOH, before and after implementing heat recovery, is calculated, and analysed for three different scenarios, as shown in Table 7, depending on the load factor (LF) of various sources and electricity costs, to demonstrate a variety of representative cost estimations.

a) Electricity from dedicated offshore wind

Table 6
Technical and cost assumptions for LCOH calculations.

Parameter	Unit	Value	Reference
Plant size	MW	10	
Lifetime of PEM electrolysis plant	Years	30	[36]
Availability/Maximum load factor	%	98	[36]
PEM stack lifetime	Years	11	[36]
Electricity Price – Offshore wind	£/kWh	0.057	[37]
Electricity Price - Grid retail price	£/kWh	0.1240	[38]
Electricity Price - Average Price Industry Sector	£/kWh	0.1814	[39]
CAPEX – PEM Electrolysis	£/kW installed	500	[36]
OPEX – PEM Electrolysis	£/kW/year	32.38	[36]
PEM stack replacement cost	£/kW installed	240	[36]
Compression (200 bar) – CAPEX	£/kg	2.49	[40]
Compression (200 bar) – OPEX	%CAPEX	6	[36]
Energy required for compression	kWh/kg	0.399	[40]
ORC – CAPEX	£/kW	358,881.6	[41]
ORC - OPEX	£/kWh	0.025	[41]
Scenario A: Dedicate offshore wind	Load Factor (%)	51	[35]
Discount rate	%	3	[42]

Table 7
Electricity prices and load factors for LCOH.

	Price (£/kWh)	Load factor (LF)	Operating hours (hrs/year)
Dedicated offshore wind electricity	0.057	51%	4,467.6
Grid electricity - industrial sector retail price	0.124	90%	7,884
Grid electricity - industrial sector average price	0.1814	98%	8,584.8

Using energy from a dedicated source means that the PEM electrolysis plants are directly connected to the electricity generation source. The source and the electrolysis process operate at an identical load factor. Dedicated energy production sources include renewable energy sources like offshore and onshore wind, solar or any combination of these. This scenario focuses on dedicated offshore wind due to its higher load factor in contrast to other renewables [35].

In this scenario, the electrolysis plant electricity price is assumed to be the levelised cost of offshore wind power generation, 0.057 £/kWh, published in the UK 2020 Electricity Generation Cost Report [37]. The load factor for offshore wind is set to be 51% [35], which means that the PEM electrolysis plant will operate 4,467.6 hrs a year.

b) Grid electricity

A PEM electrolysis hydrogen production plant may operate at a continuous and high load factor when using grid electricity. The maximum availability or load factor that can be achieved is 98% [36]. The analysis for the LCOH using grid electricity showcases two electricity prices: the industrial-sector retail price and the industrial-sector average electricity price. The industrial-sector retail pricing is based on the supposition that the hydrogen production plant is sufficiently large to join the electricity transmission grid and that its electricity policy costs are comparable to those experienced by other industrial consumers. Industrial users have lower fees than other customers, like households and businesses. This scenario assumes an electricity price of 0.124 £/kWh [38] and a load factor of 90%. The second grid-electricity scenario considers an average industrial-sector electricity price of 0.1814 £/kWh [39] and the maximum possible load factor, which is 98%. Both grid electricity prices are published by UK BEIS.

5.2. LCOH utilising electricity from offshore wind

Fig. 11 shows the levelised cost estimates of the system before and

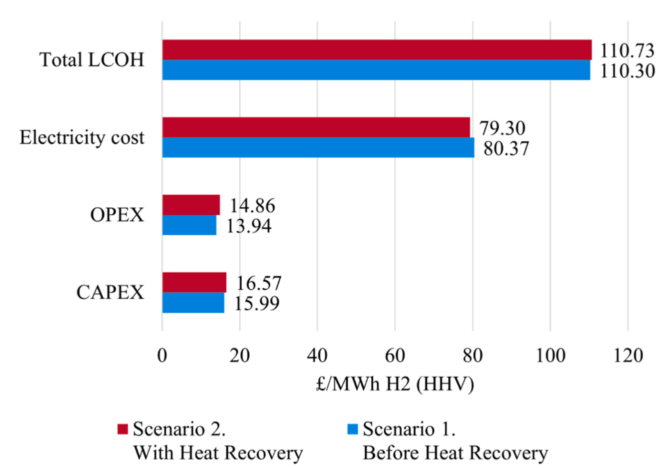

Fig. 11. Levelised Cost Estimates (£/MWh H_2 (HHV)) for 10 MW PEM Electrolysis System using offshore wind electricity.

after applying the waste heat recovery. The most significant LCOH component is the electricity cost, accounting for around 73% of the total LCOH. It can be seen that the LCOH is 110.30 £/MWh, and when implementing the waste heat recovery, the LCOH increases to 110.73 £/MWh. This means an increment of 0.43 £/MWh when implementing heat recovery and ORC. The CAPEX and OPEX are higher due to the additional costs related to the ORC system needed to produce the electricity to power the hydrogen compression process. While the purpose of implementing the heat recovery system is to generate electricity costs savings, this scenario suggests that these savings are not enough to outweigh the additional CAPEX and OPEX costs associated with the ORC.

The load factor (LF) for offshore wind is expected to rise from 51% in 2020 to 57% in 2030, and up to 63% in 2040–2050 [35]. The load factor is an important contributor to the LCOH because it impacts the operating hours of the system, which at the same time has a direct effect on the annual hydrogen production. It can be analysed from Equation (7) that higher hydrogen production will result in a lower LCOH. This effect is also presented in Fig. 12, where the LCOH for the system with heat recovery goes from 110.7 £/MWh when the LF is 51% and decreases to 106.3 £/MWh when the LF is 63%. This means an expected reduction of 4.5 £/MWh in the LCOH, with the current offshore wind load factor as a reference to the predicted load factor in 2040–2050.

5.3. Comparison of LCOH for the different scenarios

The levelised cost of hydrogen of the 10 MW PEM electrolysis plant using different electricity sources, load factors, and electricity costs is presented in this section. Table 7 summarizes the key parameters for each scenario, including the electricity prices.

As depicted in Fig. 13, utilising grid electricity at an average industrial-sector price results in the highest LCOH, while using offshore wind electricity gives the lowest LCOH. The electricity cost is the most significant component of the LCOH, and it varies depending on the electricity source. To quantitatively illustrate the variation of LCOH with electricity prices, it can be observed that the LCOH with offshore wind electricity is 110.73 £/MWh, while for industrial-sector retail price grid electricity and industrial-sector average electricity price, the LCOH is 203.94 £/MWh and 283.80 £/MWh, respectively. This represents an increment of 93 £/MWh or 84% for the retail price grid electricity scenario and 173 £/MWh or 156% for the industrial-sector average electricity price, compared to the lowest LCOH obtained with offshore wind electricity.

Even though grid electricity has a higher load factor than offshore wind, the electricity cost doubles the one for offshore wind, as shown in Table 7, resulting in an increase in total costs of the system and causing the LCOH to rise. However, when comparing the LCOH before and after implementing the heat recovery for each case, we can see that at higher electricity prices, which is the case for grid-electricity scenarios, the LCOH becomes lower when implementing heat recovery. This suggests that at higher electricity prices, it becomes more attractive and economically viable to implement the heat recovery system coupled with the ORC. This is because the electricity cost savings generated by the heat recovery system become more significant than the increase in CAPEX and OPEX related to the ORC. Therefore, to lower the LCOH, it is crucial to consider electricity prices when selecting the electricity source for the electrolysis plant.

6. Conclusions

This study presents a standardised 2-MW Proton Exchange Membrane (PEM) electrolyser model with integrated heat recovery. The developed model aligns with current commercial technologies and allows for simulating different PEM electrolysis plant sizes by aggregating as many electrolysers as necessary to reach the desired capacity. Five electrolysers were grouped together to simulate a 10-MW PEM electrolysis plant with a hydrogen production of 181.3 kg/h, equivalent to 7,143.2 kW (using H_2 HHV).

The cooling system extracts the excess waste heat as hot water at 76 °C, which is channelled to an ORC. The ORC is used for additional electricity generation to drive the mechanical compression of hydrogen. The technical analysis demonstrates that by implementing waste heat recovery coupled with ORC, the first-law efficiency of the system increases from 71.4% up to 98% (considering the thermal and electrical

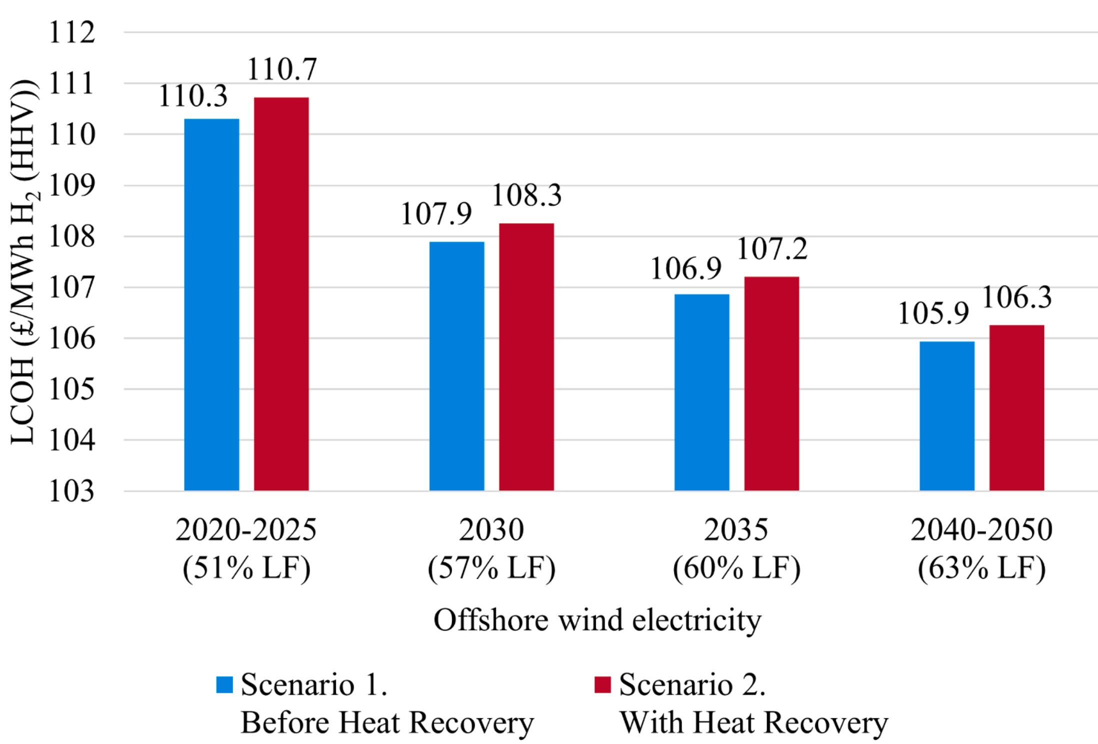

Fig. 12. Levelised Cost of Hydrogen for 10 MW PEM electrolysis system with offshore wind electricity and different load factors.

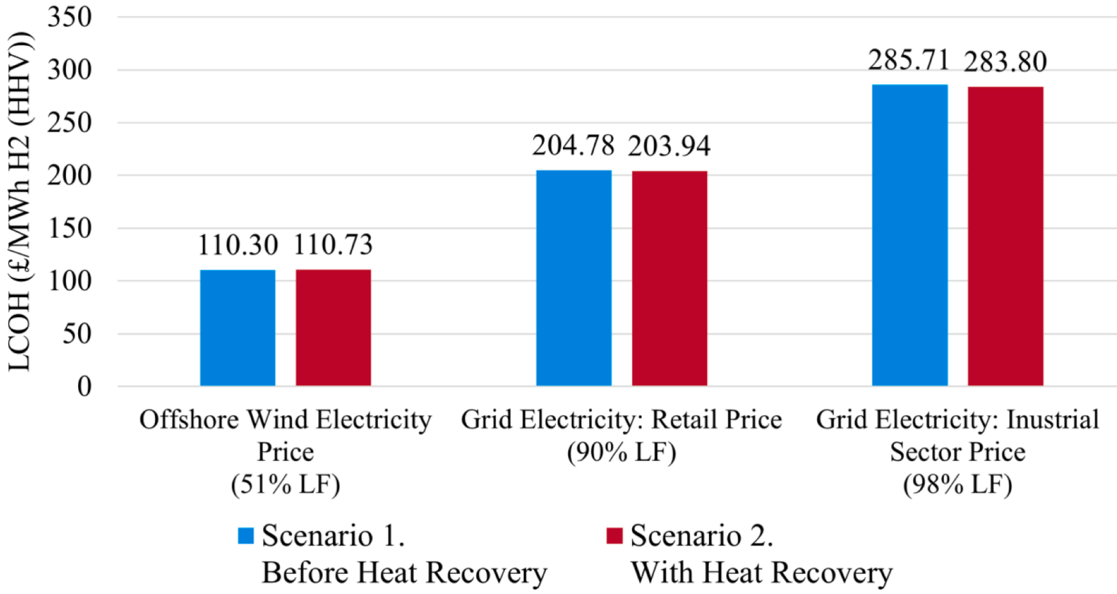

Fig. 13. Comparison of LCOH with different electricity sources.

conversion efficiencies). The results show that the ORC can completely cover the power requirement (202 kW) for compressing hydrogen from 30 bar, which is the outlet pressure at the electrolyser, up to 200 bar. When compressing hydrogen to 350 bar and 700 bar, the power generated by the ORC is insufficient, and an additional 6 kW and 100 kW are needed, respectively.

In addition, an economic analysis was conducted to calculate the system's LCOH and assess the feasibility of implementing waste heat recovery coupled with ORC to power the hydrogen compression at 200 bars. The economic analysis reveals that electricity prices dominate the LCOH. When using offshore wind electricity, which has a low electricity price (0.057 £/kWh), the LCOH is increased by 0.43£/MWh when implementing heat recovery and ORC. The findings indicate that waste heat recovery coupled with ORC is not viable for low electricity prices due to the additional CAPEX and OPEX costs incurred when implementing the ORC. In the case of cheap electricity prices, the costs of the ORC outweigh the savings generated by not purchasing electricity for compression. The results demonstrate that the opportunity and economic viability for waste heat recovery coupled with an ORC appear when electricity gets more expensive, which is the case of grid electricity prices. The results also show that the load factor is an important contributor to the LCOH. An increase in the load factor will decrease the LCOH when analysing different scenarios with varying load factors and the same electricity price.

Ultimately, the techno-economic analysis shows that when implementing waste heat recovery coupled with ORC, we get a more efficient system overall but with no economic benefit at low electricity prices. However, when the price of electricity is higher, the waste heat recovery and ORC turn out to be economically viable and more attractive.

CRediT authorship contribution statement

Ana María Villarreal Vives: Methodology, Software, Investigation, Writing – original draft. **Ruiqi Wang:** Investigation, Software, Writing – review & editing. **Sumit Roy:** Conceptualization, Supervision, Writing – review & editing. **Andrew Smallbone:** Supervision, Funding acquisition, Resources, Writing – review & editing.

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.

Data availability

Data will be made available on request.

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