

Techno-economic analysis of direct air carbon capture and hydrogen production integrated with a small modular reactor

Brittney Slavin, Ruiqi Wang, Dibyendu Roy^{*}, Janie Ling-Chin, Anthony Paul Roskilly

Department of Engineering, Durham University, Durham, DH1 3LE, United Kingdom

HIGHLIGHTS

- A sustainable energy system that combines direct air carbon capture and hydrogen production has been proposed.
- Thorough techno-economic analyses provide valuable insights into its feasibility and potential.
- By 2050, projected levelised costs are \$40/tCO₂ for carbon capture and \$1.50/kgH₂ for hydrogen production.
- A comprehensive cost comparison offers valuable benchmarks against competing technologies.

ARTICLE INFO

Keywords:

Hydrogen
Direct air capture
Electrolyser
Techno-economic analysis
Energy system

ABSTRACT

This study aims to explore the techno-economic potential of harnessing waste heat from a Small Modular Reactor (SMR) to fuel Direct Air Carbon Capture (DACC) and High Temperature Steam Electrolysis (HTSE) technologies. The proposed system's material flows, and energy demands are modelled via the ASPEN Plus v12.1 where results are utilised to provide estimates of the Levelised Cost of DACC (LCOD) and Levelised Cost of Hydrogen (LCOH). The majority of thermal energy and electrical utilities are assumed to be supplied directly by the SMR. A sensitivity analysis is then performed to investigate the effects of core operational parameters of the system. Key results indicate levelised costs of 4.66 \$/kgH₂ at energy demands of 34.37 kWh/kgH₂ and 0.02 kWh/kgH₂ thermal for HTSE hydrogen production, and 124.15 \$/tCO₂ at energy demands of 31.67 kWh/tCO₂ and 126.33 kWh/tCO₂ thermal for carbon capture; parameters with most impact on levelised costs are air intake and steam feed for LCOD and LCOH, respectively. Both levelised costs, i.e., LCOD and LCOH would decrease with the production scale. The study implies that an integrated system of DACC and HTSE provided the best cost-benefit results, however, the cost-benefit analysis is heavily subjective to geography, politics, and grid demand.

1. Introduction

1.1. Motivation

Greenhouse Gas (GHG) emissions, of which are released through the combustion of fossil fuels, are a predominant contributor to climate change [1]. The majority of GHG emissions can be attributed to CO₂, making up around 75% of total emissions, reaching 33.8 bt (419 ppm) in 2022 and is set to rise [1,2]. Of these figures, the power sector, electricity generation, and heat generation contribute to 40% of CO₂ production [3]. This presents an incentive to decarbonise such sectors. Carbon capture technologies exist today and are typically employed to mitigate carbon emissions from specific processes in isolated conditions,

i.e., from point sources. These strategies are commonly found in industrial processes such as steel and cement production, or from the scrubbing of flue gas, and can occur pre or post-combustion [4,5].

In this context, Direct Air Carbon Capture (DACC) offers the potential to achieve a net-zero carbon future by extracting CO₂ directly from the atmosphere, irrespective of emission sources. The technology can store the captured CO₂ underground or use it as a climate-neutral resource, addressing emissions from various sectors such as heavy industry, energy and transportation while removing atmospheric CO₂ [6]. However, DACC is associated with high costs, exceeding those of other CO₂ capture technologies [7]. These costs depend on factors such as the capturing technology used, energy expenses, plant configuration, and other economic parameters [6]. Currently DACC technology is still in

^{*} Corresponding author.

E-mail address: dibyendu.roy@durham.ac.uk (D. Roy).

<https://doi.org/10.1016/j.apenergy.2023.122407>

Received 2 August 2023; Received in revised form 23 October 2023; Accepted 20 November 2023

Available online 1 December 2023

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infancy and hence current techno-economics of the systems exhibit large degrees of ambiguity. The novelty of said systems arises from their ability to remove atmospheric carbon from non-centralised, hard to abate sectors, such as the transport sector which accounted for approximately 25% of global emissions in 2020 [2,8]. Hence, DACC is presented as a crucial method for achieving net-zero. The journey to net-zero requires alternative fuel sources to phase out fossil fuel use — one popular area of research for this is the use of hydrogen. The calorific content of hydrogen and its lack of emissions when combusted makes it an attractive option to satisfy future energy demands across sectors such as power, heating, and transport [9]. However, the vast majority of hydrogen production is sustained through polluting processes and hence a new method of large-scale hydrogen production must be investigated if it is to be mass produced in a net-zero scenario [10]. In this context, hydrogen production through electrolysis could play a significant role. This process involves the use of an electric current to split water into its constituent elements, hydrogen and oxygen, both of which are non-polluting. Electrolysis technologies can be broadly categorised based on their operating temperatures, namely Low-Temperature Steam Electrolysis (LTSE) and High-Temperature Steam Electrolysis (HTSE) [11]. HTSE technology, particularly solid oxide electrolyser, is suitable for cogeneration opportunities due to the availability of a higher amount of waste heat. However, solid oxide electrolysis technology faces challenges in relation to stability and degradation [12], these issues must be addressed before considering large-scale commercialisation. Small Modular Reactors (SMR) are classified as nuclear reactors with an output of less than 300 MW or 1000 MW [13]. The reactors are an attractive option over classic fossil fuel powered plants due to their smaller size and modular capabilities, making them more versatile in their construction and application. The high heat outputs of SMRs make them viable fuel sources for powering DACC and hydrogen production as secondary processes. Henceforth, if waste-heat from SMR workings can be harnessed and repurposed for the aforementioned processes, there is a possibility for net negative cogeneration to occur, where system efficiencies have the potential to reach 90% [14]. These power plants are novel but not yet mature enough for industrial rollout.

1.2. Literature review

Despite being in its early stages, DACC has made significant advancements in recent years and is a highly dynamic field of study. By 2030, it is predicted that annual CO₂ capture could increase by over 700 times current capture rates, reaching 5.5 MtCO₂/yr by 2030, and a total of 44.2 MtCO₂/yr including early development projects [15]. Funding for this sector has reached around \$180 million in private investment and \$170 million from public sources for research and development [16]. Capture costs for DACC vary widely and are heavily influenced by the type of DACC technology utilised; price ranges are often quoted to be 100–1000 \$/tCO₂, but can be narrowed down to 134–344 \$/tCO₂ according to the IEA [16]. Atmospheric carbon is still accumulating and hence nonpoint source removal processes are required — this is the appeal of DACC methods. Employing such systems can help facilitate the production of green fuels such as hydrogen and further contribute to achieving net-zero ambitions. DACC technologies can be classified into two major categories: High Temperature (HT) and Low Temperature (LT) technologies. This typically refers to Liquid DACC or Solid DACC, respectively. When identifying the technologies based on their makeup, systems can be classified as strong base aqueous solutions, amine adsorptions, and inorganic solid sorbents [17]. High Temperature (HT) DACC typically refers to systems which utilise basic or alkaline solutions, typically operating between temperatures of 300–900 °C for the regeneration process, depending on system parameters [17]. Because of this, energy demand within the system predominantly originates from heating requirements. Despite there being a limited number of DACC companies to date, Carbon Engineering are commonly cited as utilising HT DACC technology with hydroxide sorbents, namely potassium

hydroxide (KOH), in their in-development commercial DACC plant [18]. The setup comprises of four major units: the air contactor, pellet reactor, slaker, and calciner. The estimated carbon intake for this project is stated to be 1MtCO₂/yr where continuous operation is assumed and a resultant levelised cost of CO₂ captured is stated to be in the range of 94–232 \$/tCO₂ [17]. However, this financial estimation has been criticised by both industry and academic professionals as being too optimistic, where alternative values of 600–1000 \$/tCO₂ are suggested as a more realistic pricing range [19].

A benefit of HT DACC compared to its Low Temperature (LT) counterpart is the system's ability to withstand degradation of its contactor and thus requires less spending for replacing parts [20]. This drastically extends the lifetime of the plant and helps reduce operating expenditure (OPEX). Conversely to HT DACC, LT DACC is predominantly comprised of a solid adsorbent operating under low pressure and requires lower temperatures to facilitate regeneration. Hence, a reduced heat demand is exhibited which contributes to cheaper operating costs [8]. Because of these features, this technology is often the predominant suggested method to harness low-grade waste heat to power its processes [21]. The general make-up of LT DACC is an amine base that is bonded to a porous structure - industry examples of such setups are demonstrated by Climeworks [22] and Global Thermostat [23].

As mentioned previously, LT technology is typically more affordable compared to HT DACC and is reflected in the pricing estimations of around 233 \$/tCO₂ when fuelled from nuclear waste heat [24]. However, price ranges can be affected by the choice of energy source for the system, the system scale, and the location of the plant itself; these factors also apply to HT DACC. From these variables and the differing economical and energy consumption assumptions, values quoted from various literature for LT DACC range from 75 to 730 \$/tCO₂ [8,25]. Although cheaper on average, the OPEX associated with having to replace the physical contactor does impact the project's financials over an extended period of time [20].

Global hydrogen production is estimated at 75 Mt., equating to 9 EJ/yr [9]. Narrowing the scope to Europe, the future continental demand is predicted to reach 16.9 Mt. by 2030, with approximately 49% expected to be produced from electrolysis-based methods with carbon capture, 44% from electricity supplied by renewable energy sources, and 7% from coal gasification [9]. However, despite the various technologies available, 96% of global hydrogen production is produced via fossil fuel powered methods, of which steam methane reforming is most prevalent [26]. Current methods therefore contribute to a significant amount of CO₂ production where an average of 889 MtCO₂ was released between 2019 and 2021 resulting in an average emission intensity of 9.7 gCO₂/gH₂ across the range given [10]. Hence, hydrogen production technologies are now subject to new growth catalysed by the increase in demand for alternative and sustainable fuels as well as energy storage options [9]. Hydrogen as an energy store is being explored to harness excess nuclear power that is produced due to fluctuations in grid demand. This can allow for a more versatile energy network, particularly as renewables become increasingly incorporated to satisfy energy demands, and hence less energy wastage. Furthermore, many initiatives revolving nuclear-hydrogen cogeneration are being pushed forward to allow for clean power and hydrogen production — of note is the UK's plan to implement 10 GW of low-carbon hydrogen production capacity by 2030 [27]. The majority of such investigations are in preliminary stages and so are not commercially viable. Nevertheless, low-carbon hydrogen production demand is present and nuclear cogeneration is becoming an increasingly attractive option due to its stable operation. Ideas of incorporating renewable energy sources to assist in production, such as wind, are also being explored, although volatility of such sources presents difficulties when considering their incorporation into current energy infrastructure.

Hydrogen production technologies are well established in industry. Key methods include: electrolysis with varying electrolyzers (Alkaline, Polymer Electrolyte Membranes, Solid Oxide), natural gas reforming,

biomass gasification, biomass derived liquid reforming, and solar thermochemical hydrogen [28]. Of these methods, only electrolysis-based production and solar thermochemical splitting provide the framework for carbon offsetting of hydrogen. Investigations on utilising industrial waste heat to partially fuel HTSE have been explored in the literature. HTSE functions by splitting water into hydrogen and oxygen via solid oxide electrolysis cells where process heat is typically used to reduce the amount of electricity utilised [29]. Operating temperature ranges have displayed small variation in the literature, with the overall operating range within 750–1000 °C [30,31]. Although pure hydrogen is desired in some cases, the production of hydrogen is being explored in conjunction with carbon dioxide usage to diversify the products produced. This pairs the production of hydrogen with DACC to propose a beneficial working relationship, facilitating the production of alternative fuels and industry process materials such as ammonia [32].

Limited research has been conducted on directly utilising the waste heat from SMR processes for alternative production methods, though this area presents promising opportunity in assisting in worldwide decarbonisation and exploring more effective uses of SMR technology. Literature data does support the notion that waste heat from a high temperature SMR would be sufficient in powering the additional processes of DACC and HTSE. From this, the overall system efficiency has potential to reach 90% and beyond, assuming that the majority of waste heat can be harnessed effectively [10]. This is particularly promising when considering the constant annual operation of the reactor and the fluctuation in public energy demand from the grid. During off-peak hours, the reactor is supplying more than the required demand; taking the opportunity to utilise this additional energy towards CO₂ extraction and hydrogen production presents the possibility of increasing plant revenue as the output materials could be sold or repurposed further into other sought after goods. Such goods would be dependent on market demands.

Hydrogen production systems have been studied and documented in literature. For instance, Hosseini [33] investigated a hybrid system integrating a gas turbine (GT) fuelled by biogas, complemented by a solid oxide electrolyser subsystem for hydrogen generation. The findings illustrated that through the purification of biogas and the increase of CH₄ concentration to 80%, the hybrid system would generate more electrical power by 24% and produce more hydrogen by 20%. Assareh et al. [34] analysed the techno-economic performance of a hybrid system which integrated photovoltaic thermal (PVT), absorption chiller, organic Rankine cycle and polymer electrolyte membrane (PEM) electrolyser. Their system would achieve the highest hydrogen production rates, reaching approximately 0.25 kg/h with an estimated cost of 1.29 \$/kWh. Wang et al. [35] investigated the techno-economic performance of a cogeneration system which integrated plasma gasification, methanol synthesis, supercritical CO₂ cycle and alkaline electrolyser. They reported that their proposed system could recover the initial investment in just 3.53 years, and over its 20-year operational lifespan, the waste-to-energy project could generate a net present value of 355,318.47 k\$. Locatelli et al. [36] assessed the feasibility of incorporating SMR with alkaline electrolyser, HTSE and sulphur-iodine cycle. They indicated that operating an alkaline electrolyser facility would become economically viable when the selling price of hydrogen reached or exceeded €0.40 per Nm³. Coppitters et al. [37] conducted a sensitivity analysis on hydrogen production by integrating PEME with a photovoltaic system under various climatic conditions. Their findings revealed that the levelised cost of hydrogen would range from 6.3 €/kg to 10.5 €/kg, showcasing the variability across different scenarios. Bhandari and Shah [38] conducted a techno-economic evaluation of integrating solar photovoltaic with alkaline electrolysis and PEME in both grid-connected and off-grid configurations. They reported that the most cost-effective approach for hydrogen production would be the grid-connected solar photovoltaic system combined with alkaline electrolysers, offering 6.23 €/kg as the levelised cost of hydrogen (LCOH). Yilmaz [39] investigated techno-economic analysis of a hybrid system integrating a combined

flash-binary geothermal power plant with alkaline electrolyser for hydrogen production. Their cost of electricity and hydrogen were estimated as 0.01066 \$/kWh, and 1.088 \$/kg, respectively. Bhattacharyya et al. [40] integrated a stand-alone photovoltaic energy system with an alkaline electrolyser for hydrogen production, considering real-world ambient conditions. Their annual average hydrogen production rate was estimated as 10.5 Nm³/h.

1.3. Novelty and contribution

Table 1 summarises previous studies related to DACC. The concept of combining waste heat for DACC and hydrogen production has not been fully explored, thus research regarding technical feasibility as well as cost analysis for such designs is required. While various established methods exist for hydrogen production with associated costs, this is not the case for DACC as ranges are vast and unreliable, nor is there sufficient techno-economic data available for such an integrated system. Through an extensive review of the existing literature and to the best of the authors' knowledge, it is evident that no techno-economic study exploring the production of hydrogen using a HTSE, alongside the integration of a DACC facility with a SMR, exists in the literature. Henceforth, this paper aims to explore the techno-economic plausibility of an integrated DACC and HTSE hydrogen production system powered by SMR, and various scenarios are investigated to assess its feasibility.

A proposed schematic highlighting potential avenues for hydrogen production and carbon capture is highlighted in Fig. 1, with circled areas highlighting areas of interest for this study. The majority of waste heat will be categorised in the medium to high grade range, making it a suitable source for fuelling LT and HT DACC, as well as HTSE for additional hydrogen production. Electrical energy demands can be harnessed from the primary energy output of the SMR, allowing for optimised operational efficiency and better system assimilation. The major contributions of the study are listed below:

- Conceptualisation of an integrated system comprising small modular reactors, DACC, and HTSE technologies.
- Techno-economic assessment of the proposed system has been performed.
- Comparison of levelised costs across different technologies and various scenarios has been performed.
- Sensitivity analysis has been conducted, and levelised costs are projected up to the year 2050 scenario.
- The study sheds light on the cost-competitiveness of the proposed integrated system in the current context and discusses potential future scenarios, envisioning a reduction in costs as climate policies become stricter and demand for these technologies increases.

1.4. Organisation

In Section 2, “materials and methods,” the system description and the techno-economic modelling of the proposed energy system are detailed. Section 3 presents the results of the study, while Section 4 includes discussions covering technical and economic data analysis, implementation, market behaviour, and the exploration of future work. Finally, Section 5 offers the conclusion of the study.

2. Materials and methods

The investigation can be categorised into two primary parts, of which the first facilitates the other. The first section looks into modelling of the system utilising the leading process simulation software ASPEN Plus v12.1. The second section delves into the economic calculations of the simulated plant, where this data is then compared to data found in literature to evaluate the validity of results.

Table 1
Previous DACC integrated studies found in the literature.

Ref	System configuration	Methods	Major results
[41]	• DACC, PEM electrolyser, and methanation unit	Thermodynamic, economic, and environmental analyses	<ul style="list-style-type: none"> The exergy efficiency ranges from 51.3% to 52.6%. The levelised cost of synthetic natural gas ranges from 130 €/MWh to 744 €/MWh.
[42]	• DACC with CO ₂ utilisation employing HTSE	Economic analysis	<ul style="list-style-type: none"> The levelised cost is reported as 382 \$/t CO₂.
[43]	• DACC, Solid Oxide electrolyser, and electric grid	Technical analysis	<ul style="list-style-type: none"> The start-up time from hot-standby to 70% of nominal load decreased by a factor of five times.
[32]	• DACC, ammonia production • DACC and methanol production	Economic study	<ul style="list-style-type: none"> The ammonia-based infrastructure exhibits the lowest levelised cost of energy transmission, amounting to \$10.1 per gigajoule (GJ).
[44]	• DACC, PEM electrolyser, and CO ₂ -based alternative fuel production	Technical and economic analyses	<ul style="list-style-type: none"> Methanol, dimethyl ether (DME), and methane fuel systems exhibit hydrogen-to-fuel energy efficiencies of 88.4%, 85.2%, and 83.3%, respectively, along with exergetic efficiencies of 92.9%, 92.1%, and 86.2%. The costs of storage for methane, methanol, and DME fuel pathways are found to be 0.239 \$/kWh, 0.251 \$/kWh, and 0.244 \$/kWh, respectively.
[45]	• DACC integrated with heating, ventilation and air conditioning (HVAC) system	Thermodynamic study	<ul style="list-style-type: none"> The optimal exergy efficiency is 81.9%, and the coefficient of performance (COP) is 7.21.
[46]	• DACC powered by natural gas combined cycle (NGCC) plant and post combustion carbon capture	Techno-economic analyses	<ul style="list-style-type: none"> A CO₂ price ranging from \$150 to \$225 per tonne is necessary to achieve a positive net present value (NPV).
[47]	• DACC based on algae-based coating	Techno-economic analysis	<ul style="list-style-type: none"> The carbon removal efficiency ranges from 44% to 51%, while the sequestration costs range from \$702 to \$1585 per tonne of CO₂.
[48]	• DACC using Two conventional adsorption processes, Vacuum-pressure swing adsorption (VPSA) and temperature-vacuum swing adsorption (TVSA) cycles	Thermodynamic analysis	<ul style="list-style-type: none"> The optimal exergy efficiencies for SIFSIX-3-Ni, NbOFFIVE-3-Ni, N₂H₄/Mg-MOF-74, TRI/PE-MCM-41, and DETA/PPN-6 are 32.5%, 43.9%, 50.5%, 49.5%, and 50.9%, respectively.
[49]	• DACC+ heat recovery+ Electrolyser	Technical analysis	<ul style="list-style-type: none"> At an equilibrium cell voltage of 1.5, excess heat production amounts to 475 kJ per mole of captured CO₂.

2.1. System description

A simplified overview of the system setup is displayed in Fig. 2. The proposed system for this paper comprises of a high temperature small modular reactor of 36% thermal efficiency. The efficiency value coincides with the modal range of SMR efficiencies and represents the mean thermal efficiency from the listed reactors suggested in [21]. It is important to note that additional heating in the calciner would be required to bring the SMR steam temperature up from 800 °C to the required 900 °C; modelling this with a Supplementary Heater block utilising nuclear-generated electricity would require 15,789 cal/s or around 66 kW. Furthermore, the system utilises a HT KOH solution DACC setup as well as HTSE for hydrogen production which have been modelled from Carbon Engineering's DACC setup [18]. Fig. 3 presents schematic diagrams for the HTSE model and the DACC model. The DACC model is similar to the model presented by [50] and the HTSE model is similar to the model presented by [51]. Five blocks are included in the DACC model, namely the air contactor, pellet reactor, slaker, calciner, and CO₂ compression unit. Adjustments have been made to reduce system complexity and complications when modelled with other components. Electrical demands of the system are met internally by the SMR's electricity production. These setups should theoretically be able to be facilitated via the waste heat produced from a high temperature reactor. The model was developed using the ASPEN Plus flowsheet model. The liquid phase utilised the ELECTROLYTE NRTL property method, while the gas phase employed the Soave-Redlich-Kwong equation of state (SRK-EoS) property method. A summary of the input parameters and operating conditions of both systems can be found in Table 2.

2.2. Direct air carbon capture (DACC)

The DAAC process was detailed in [17] as highlighted here. During the process, ambient air is drawn through the air contactor unit, where its CO₂ content reacts with the aqueous KOH solution to form potassium carbonate (K₂CO₃), as presented in Eq. (1). K₂CO₃ solution is then pumped into the pellet reactor, which contains calcium carbonate (CaCO₃) pellets suspended in the reactor. A slurry of calcium hydroxide (Ca(OH)₂) is injected at the bottom of the reactor, driving the dissolution of Ca(OH)₂ and the precipitation of CaCO₃, as presented in Eq. (2). CaCO₃ pellets are added at the top of the reactor. As they grow, they discharge from the bottom of the reactor to the calciner, where CaCO₃ is thermally decomposed at approximately 900 °C to yield CO₂ and calcium oxide (CaO), as presented in Eq. (3). The CO₂ stream is then compressed and cooled in the compression unit, ready to be sequestered or sold and transported. In the slaker unit, CaO is hydrated to form Ca(OH)₂, which can then be fed back into the pellet reactor, as presented in Eq. (4). The chemical reactions for the process [17] are summarised below.



2.3. High temperature steam electrolysis (HTSE)

The HTSE model considered in the analysis produces hydrogen consuming the required electricity and heat supplied by a SMR. The electrochemical reactions that occurred in the solid oxide electrolyser stack are given in Eqs. (5)–(7) [51]:



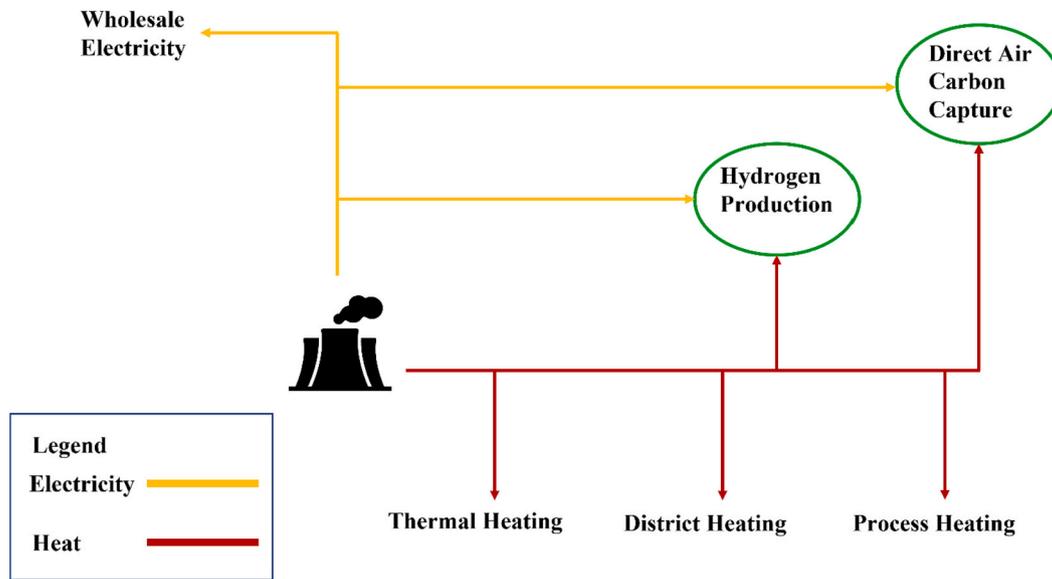


Fig. 1. Scope of the work. (Areas of interest for this study are circled in green). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

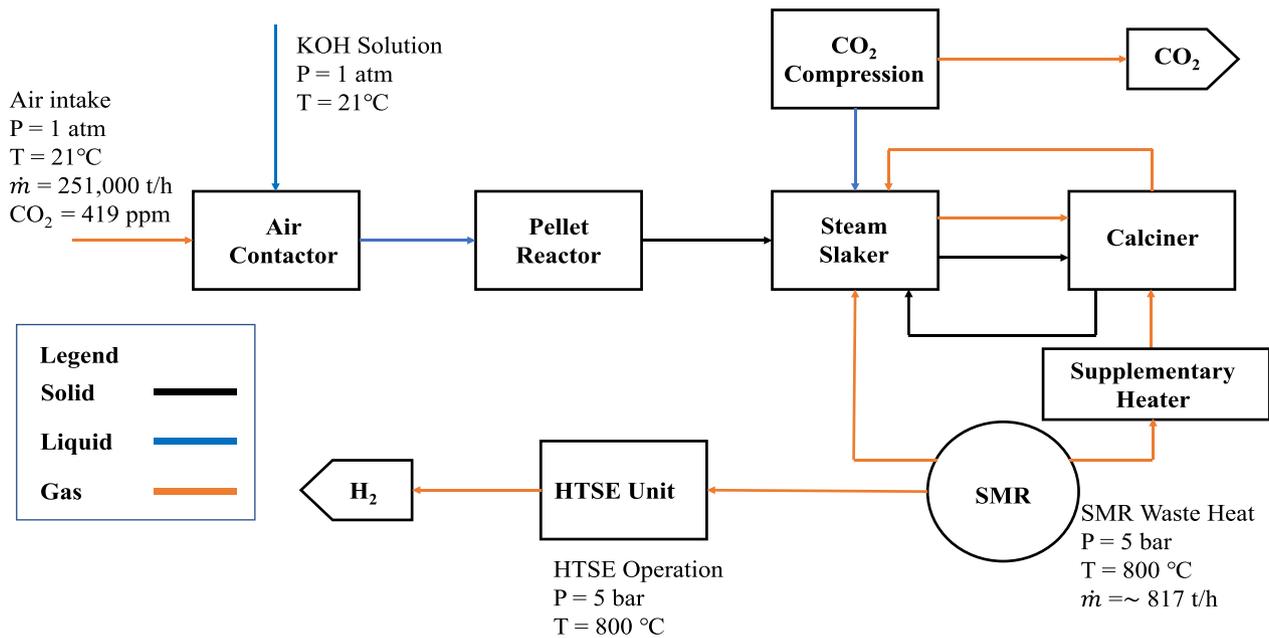


Fig. 2. Proposed system comprising of HT DACC, HTSE based hydrogen production, and waste heat from a high temperature SMR.



The Nernst voltage, E (V), can be estimated by following Eqs. (8)–(9) [51]:

$$E = E^0 + \frac{RT}{2F} \ln \left(\frac{P_{H_2} \times P_{O_2}^{0.5}}{P_{H_2O}} \right) \quad (8)$$

$$E^0 = 1.253 - 2.4516 \times 10^{-4} T \quad (9)$$

where E^0 is the standard voltage (V); R is the ideal gas constant; T is the operating temperature of electrolyser (K); F is the Faraday's constant (96,485C/mol); and P_{H_2} , P_{H_2O} and P_{O_2} are the partial pressures of

hydrogen, steam, and oxygen, respectively (kPa), which are measured using the following equations [54].

$$P_{H_2} = x_{H_2} \times P_{cell} \quad (10)$$

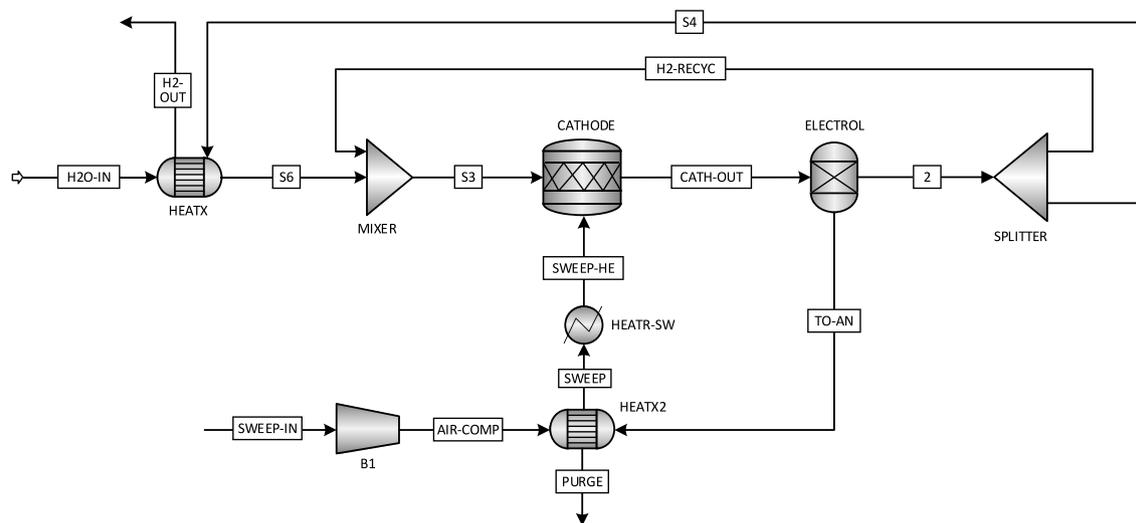
$$P_{O_2} = x_{O_2} \times P_{cell} \quad (11)$$

$$P_{H_2O} = x_{H_2O} \times P_{cell} \quad (12)$$

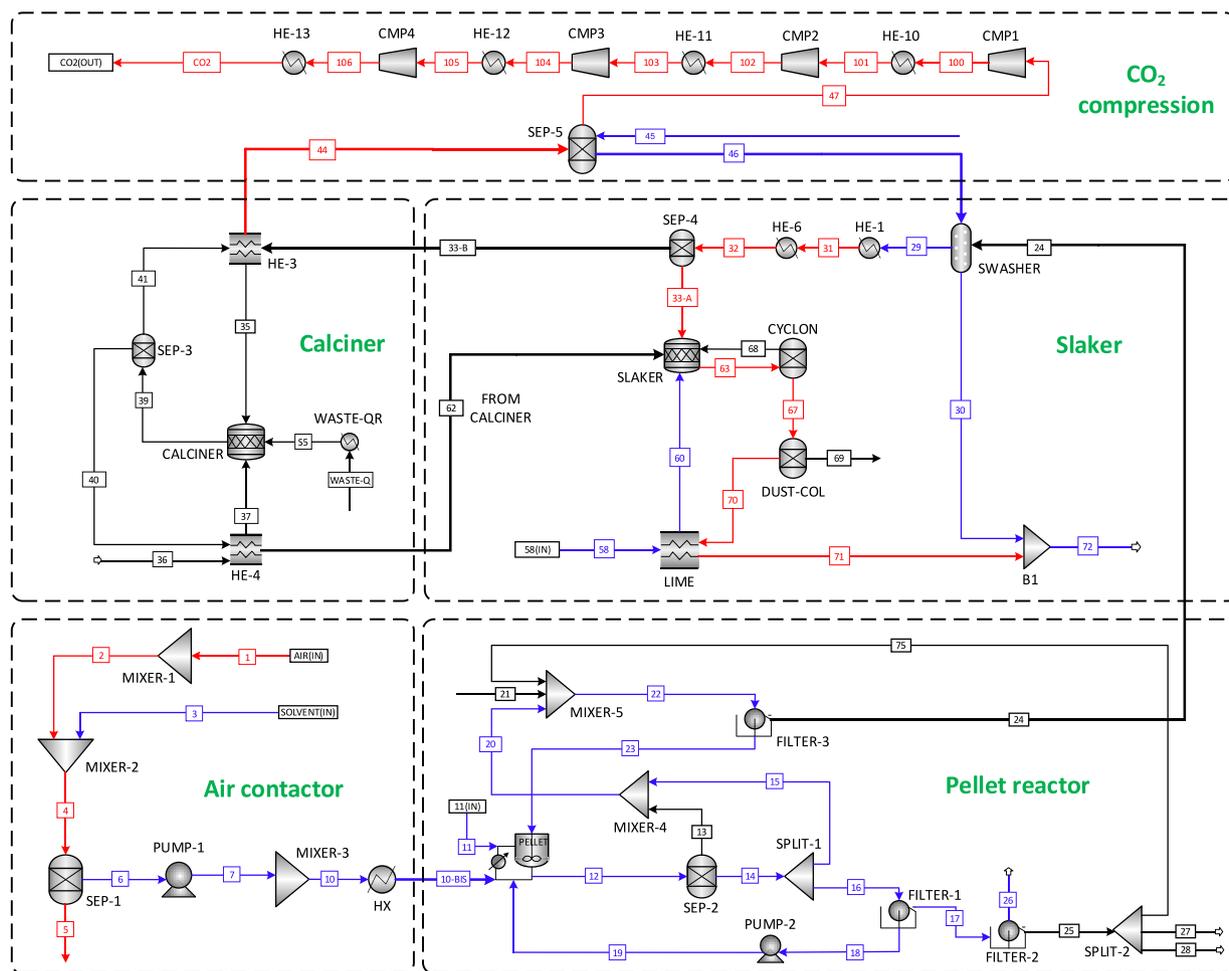
where x_{H_2} , x_{O_2} , and x_{H_2O} are molar fractions of hydrogen, oxygen, and steam, respectively. Operating pressure of the HTSE is denoted by P_{cell} . The cell voltage of the solid oxide electrolyser, V_{SOE} (V), can be estimated by using Eq. (13) [51]:

$$V_{SOE} = E + V_{ACT} + V_{Ohm} + V_{Con} \quad (13)$$

where, V_{ACT} , V_{Ohm} and V_{Con} represent activation overpotential, ohmic



(a)



(b)

Fig. 3. Schematic diagram of (a) HTSE model; (b) DACC model.

Table 2
Base case input parameters.

Sub-system	Parameter	Unit	Value	Ref.
SMR	Power Rating	MW	300	[13]
	Thermal Efficiency	%	36	[25]
	Air Intake Flow Rate	t/h	251,000	[50]
DACC	Air Intake Temperature	°C	21	[50]
	Air Intake Pressure	atm	1	[50]
	KOH Solution	t/h	4394	[50]
	Operating Temperature	°C	800	[52]
HTSE	Operating Pressure	bar	5	[52]
	Steam Utilisation Rate	%	80	[53]

overpotential and concentration overpotential, respectively (V).

The activation overpotential is the total energy loss due to chemical kinetics of the electrochemical reactions at the anode and cathode respectively, $V_{ACT,a}$ and $V_{ACT,c}$, and can be calculated by the following relations [51]:

$$V_{ACT} = V_{ACT,a} + V_{ACT,c} \quad (14)$$

$$V_{ACT,i} = \frac{RT}{F} \ln \left[\frac{j}{2j_{0,i}} + \sqrt{\left(\frac{j}{2j_{0,i}} \right)^2 + 1} \right] \quad (15)$$

$$j_{0,i} = \gamma_i \times \exp \left(-\frac{EA_{ACT,i}}{RT} \right) \quad (16)$$

where j is the current density (A/m^2), $j_{0,i}$ is the exchange current density at the anode ($i = a$) and cathode ($i = c$); γ_i is the pre-exponential factor (A/m^2), and $EA_{ACT,i}$ is the activation energy of the cathode and anode respectively ($J/mol.K$).

The ohmic overpotential, V_{Ohm} , is related to the loss due to a resistance within the electrolyte layer, which can be estimated using Eq. (17) [51]:

$$V_{Ohm} = 2.99 \times 10^5 \times j \times L \times \exp \left(\frac{10300}{T} \right) \quad (17)$$

where L is the electrolyte thickness (m).

The concentration overpotential, V_{Con} (V), can be estimated as the total concentration overpotential at the cathode and anode, $V_{Con,c}$ and $V_{Con,a}$ respectively, by following Eqs. (18)–(20) [51], which is associated by the mass transfer resistance between the electrodes and electrolyte:

$$V_{Con} = V_{Con,c} + V_{Con,a} \quad (18)$$

$$V_{Con,c} = \frac{RT}{2F} \ln \left[\frac{(P_{H_2} + jRTd_c/2FD_{H_2O}^{eff})P_{H_2O}}{(P_{H_2O} - jRTd_c/2FD_{H_2O}^{eff})P_{H_2}} \right] \quad (19)$$

$$V_{Con,a} = \frac{RT}{4F} \ln \left(\frac{\sqrt{(P_{O_2})^2 + (jRT\mu_{O_2}/2FB_G)}{P_{O_2}} \right) \quad (20)$$

where $D_{H_2O}^{eff}$, μ and B_G are effective diffusion coefficient of steam, dynamic viscosity of oxygen ($kg/(m \cdot s)$) and flow permeability (m^2), respectively.

2.4. Economic analysis

Economic evaluation will be undertaken by utilising key economic measures such as: estimations of Capital Expenditure, CAPEX (\$); Operational Expenditure, OPEX (\$); the Levelised Cost of Electricity, LCOE (\$/kWh); Levelised Cost of DACC, LCOD (\$/t); and Levelised Cost of Hydrogen, LCOH (\$/kg). Upon acquiring these values, a sensitivity analysis can be conducted to explore the impact of various operating conditions on the system and how these impact the levelised costs

derived. An analysis into the movements of the energy sector will be considered and used to assess the market competitiveness of such technologies, based upon publicly available data, in conjunction with the aforementioned economic measures. This will be used to characterise the technology readiness level of such a facility as well as establishing its place in the green energy transition.

The total life cycle costs, TLCC (\$) of the system can be estimated by Eq. 21:

$$TLCC = CAPEX + \sum_{n=0}^N \frac{OPEX_n + O\&M_n}{(1+d)^n} \quad (21)$$

where CAPEX is the Capital Expenditure costs, N is the lifetime of the system, n is the operational year, OPEX is the Operating Expenditure, O&M is the Operation and Management costs, d is the discount rate.

The Levelised cost of DACC, LCOD (\$/t) is defined by the following relation:

$$LCOD = \frac{TLCC_{DACC}}{\sum_{n=1}^N \frac{m_{CO_2}}{(1+d)^n}} \quad (22)$$

where m_{CO_2} is mass of CO₂ captured (t).

The Levelised cost of Hydrogen, LCOH (\$/kg) is defined by the following relation:

$$LCOH = \frac{TLCC_{HTSE}}{\sum_{n=1}^N \frac{m_{H_2}}{(1+d)^n}} \quad (23)$$

where m_{H_2} is mass of hydrogen produced (kg).

The capital recovery factor (CRF) can be defined by the following eq. [8]:

$$CRF = \frac{WACC(1+WACC)^N}{(1+WACC)^N - 1} \quad (24)$$

where WACC is the Weighted Average Cost of Capital.

3. Results

3.1. Technical evaluation

Key system performance metrics for both base cases of DACC and HTSE are summarised in Table 3. It indicates that a CO₂ capture rate of 112 t/h at an electrical energy demand of 3482 kW and a much larger thermal demand of 14,151.38 kW, corresponding to an electrical utility cost of 270 \$/h. This results in an estimated electrical power demand to tonne of CO₂ captured of 31.67 kWh/tCO₂. Additionally, a hydrogen production rate of 0.2 t/h at an electrical energy demand of 6880 kW and a thermal demand of 4.49 kW, equating to an electrical utility cost of 533 \$/h. Utilising the aforementioned steam feed of 1922 kg/h yields an electrical power demand to hydrogen production ratio of 34.37 kWh/kgH₂. Energy requirements and costs associated with compression have not been included in order to provide a more focused overview of the key operations of such systems - compression specifications are influenced on the intended use of the system outputs and hence would

Table 3
Summary of simulation outputs for both the HTSE and DACC units.

Parameter	Unit	Value	
		DACC	HTSE
Production / Capture Rate	t/h	112.02	0.20
Electrical Energy Demand	kW	3482	6880
Thermal Energy Demand	kW	14,151.38	4.49
Electrical Energy Cost	\$/h	269.85	532.92
Efficiency	%	–	91.31

detract from the primary energy demands of the systems if included.

Investigations regarding the CO₂ content captured in the DAC system were conducted by varying mass flow rate of the KOH aqueous sorbent being introduced into the system. This was performed by incrementally altering a Design Specification implemented in the simulation that essentially regulates the ratio between the CO₂ purged against the CO₂ introduced to the system, where the difference between these values indicates the net captured CO₂. Higher specification ratio indicates that less CO₂ is captured from the air. In the analysis, the specification ratio was varied from 0.1 to 0.9, where values beyond 0.9 yielded simulation errors. Results are highlighted in Fig. 4 along with the estimated utility demand.

Fig. 4 shows that an increase in flow rate of KOH sorbent from 0.5 to 5.6 kt/h results in an increase in CO₂ capture rate alongside power demand, where maximum CO₂ captured reached 135.5 t/h at a utility power demand of 3.49 MW. This gave a value of 25.7 kWh/tCO₂ captured. Utility pricing for the DAC system ranged from 265 to 270 \$/h; this appeared to have a positive correlation between utility pricing and mass flow rate of sorbent, and hence CO₂ captured.

A similar investigation into the hydrogen output was conducted in order to deduce a possible output range for the HTSE system, which is highlighted in Fig. 5. This was performed via a sensitivity analysis where steam feed was varied from 1000 to 10,000 kg/h. Control variables regarding the temperatures and pressures of the steam input stream and electrolyser were maintained at 800 °C and 5 bar in order to reflect the typical operating conditions as expressed in literature.

Here a positive linear correlation between steam feed, hydrogen output, and stack power demand can be identified. The maximum hydrogen generated from the simulation was recorded at 1041.9 kg/h at a steam feed of 10,000 kg/h and a resulting stack power demand of 35.8 MW, equating to 34.37 kWh/kgH₂ which is same as the specific power demand for producing 1 kg hydrogen in the base case. Moreover, utility pricing data ranged from 277 to 2773 \$/h based on an increase in steam feed.

To assess the factors affecting the specific power demand for producing hydrogen, a sensitivity analysis of steam utilisation rate was performed, and its effects on the hydrogen output and specific power demand are shown in Fig. 6. The steam input was based on the base case, i.e., 1922 kg/h at 800 °C and 5 bar. The results show that 100% conversion of steam could produce the maximum hydrogen of 215 kg/hr and reduce the power demand for producing 1 kg hydrogen to 34.36 kWh/kgH₂. Although it is difficult to achieve 100% steam feed utilisation in actual operation of the HTSE, improved steam utilisation is essential to increase hydrogen production and reduce energy

requirement.

3.2. Economic evaluation

Utilising the base case setup and equations discussed in materials and method section, key financial parameters are summarised in Table 4, along with their assumptions. Sensitivity analyses were conducted in order to explore the effect of various parameters on the calculated levelised costs to capture and produce CO₂ and hydrogen, respectively. Data has been normalised to the base case scenarios to highlight how many times more or less the levelised costs vary compared to their baselines. Results are provided via tornado plots to give a visual indication to the weight of analysed parameters on levelised costs as shown in Figs. 7 and 8. The grey bars of the tornado plots highlight a decrease from the base case parameter value and bars in red highlight an increase from said values, with the respective values used for the analysis at either end of the bars.

In Fig. 7, the DAC system appears to be heavily reliant on air intake, where less air intake results in a considerably higher LCOD. Reducing the air intake by 20% drastically increased the levelised cost of carbon capture by 13.29 times the magnitude of the base case LCOD. However, increasing the intake to 301,200 t/hr resulted in a 13% reduction in costing. This equated to levelised costs of 1650 \$/tCO₂ and 103 \$/tCO₂, respectively. Electrical utility costs and plant lifetime made minimal relative impact to costing, where electrical utility costs resulted in LCODs of 123.66 \$/tCO₂ and 124.63 \$/tCO₂. A reduction in plant lifetime to 20 years resulted in 132.49 \$/tCO₂ and 119.27 \$/tCO₂ when increased to 30 years.

From Fig. 8, it can be seen that the mass flow rate of steam feed had the largest impact on the HTSE system's economic performance, reaching a maximum deviation of 1.11 times the base case LCOH when the inlet steam is reduced by 20% of the base case steam feed, resulting in an LCOH of 5.16 \$/kgH₂. Conversely, when increased by 20%, this yielded 0.93 times the original LCOH, giving a reduced value of 4.32 \$/kgH₂. Electrical utility cost was varied by 20% either way which resulted in deviations of 11% from the original cost, where an increase in utility price resulted in an increased value of LCOH. This parameter appeared to make the least impact on levelised costs, however, it is worth noting that all parameters analysed show minimal deviation from the base case LCOH.

Further analysis on the effects of steam utilisation rate on LCOH performance is illustrated in Fig. 9. As the steam utilisation rate increases, the LCOH decreases. This phenomenon is attributed to the higher production of hydrogen associated with an increasing steam

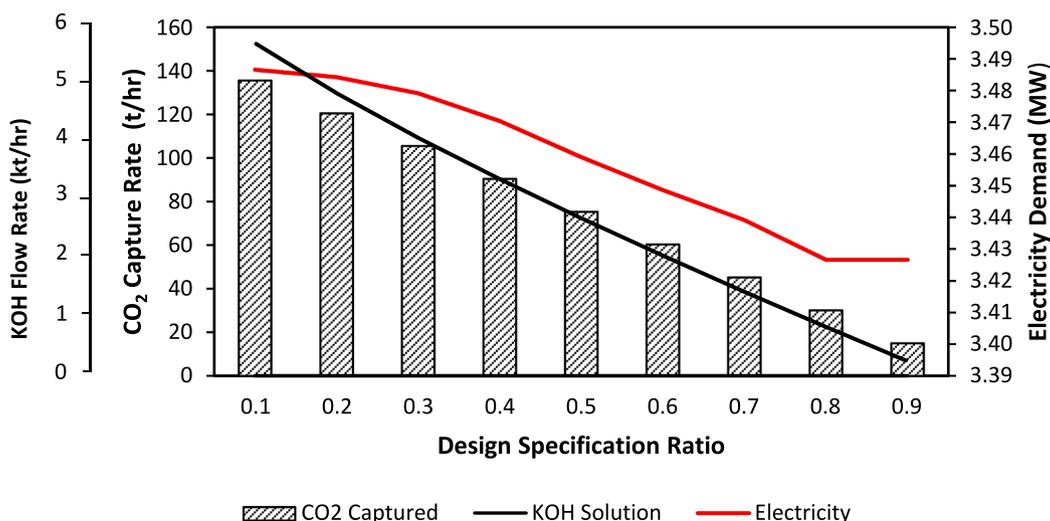


Fig. 4. Correlation between varying KOH solution and CO₂ capture rate alongside power demand.

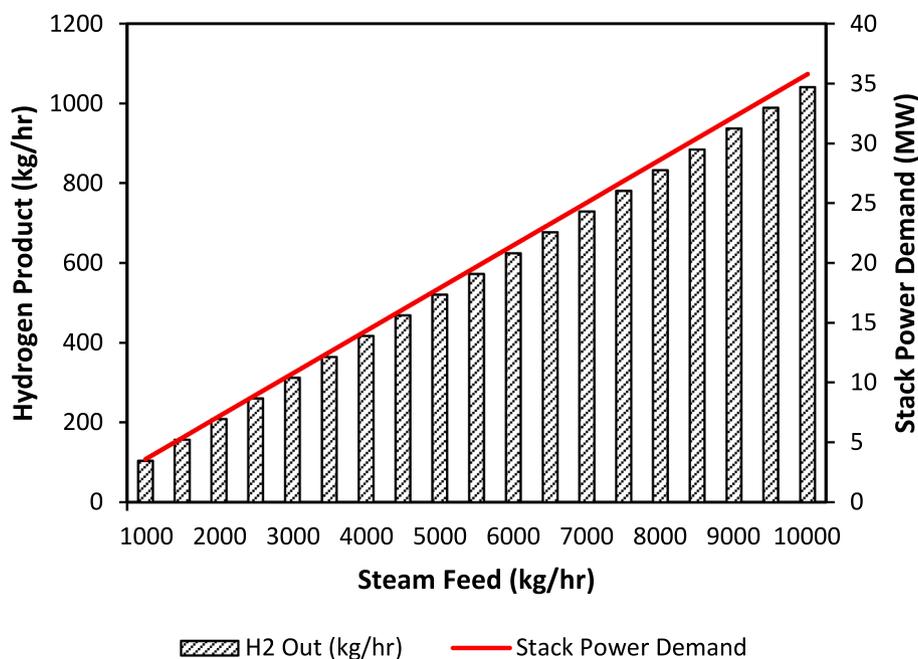


Fig. 5. Sensitivity analysis of steam feed mass flow rate and its effect on hydrogen output and energy demand of the HTSE unit.

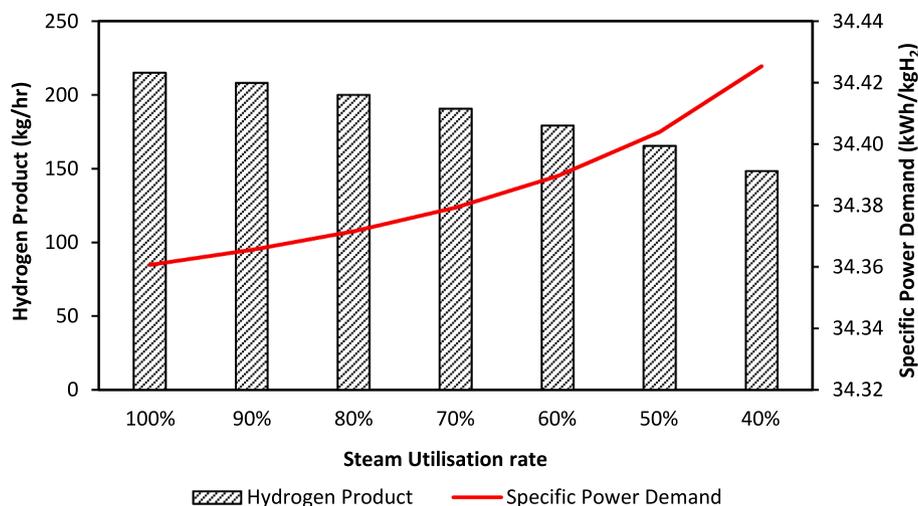


Fig. 6. Sensitivity analysis of steam utilisation rate and its effect on hydrogen output and specific power demand for producing 1 kg hydrogen.

Table 4

Estimated economic parameters assumptions for base case.

Parameter	Units	HTSE	DACC
Lifetime	yr	25	25
Production/Capture	t/yr	1752	981,321
CAPEX	m\$	28.88	1292.89
OPEX	m\$/yr	4.67	2.36
Discount rate	%	9	9
CRF	%	10.2	10.2
LCOH	\$/kg	4.66	n.a
LCOD	\$/t	n.a	124.15

utilisation rate. The minimum LCOH is estimated at a 100% steam utilisation rate, while the maximum LCOH is reported at a 40% steam utilisation rate, with values of \$4.33/kg and \$6.28/kg, respectively.

4. Discussion

4.1. Data analysis

The main caveat of this study is the heavy reliance on secondary data from various technical simulations to form the parameters for the ASPEN Plus model and the nature of economic data extrapolation - both of which produce results that are incredibly influenced by initial assumptions imposed on the studies. This is further emphasised when considering the Technology Readiness.

Level (TRL) of the analysed technologies and hence the lack of industry examples available for accurate and reliable analysis. Both technologies are mainly within a TRL range of 6–7, signifying large scale prototypes and demonstrated functionality but not to the point of maturity to be considered established within industry [8,55]. Furthermore, many studies regarding DACC analysis are based on the same reference paper published by Carbon Engineering which may limit the range of findings [17]. However, this paper is often used as the

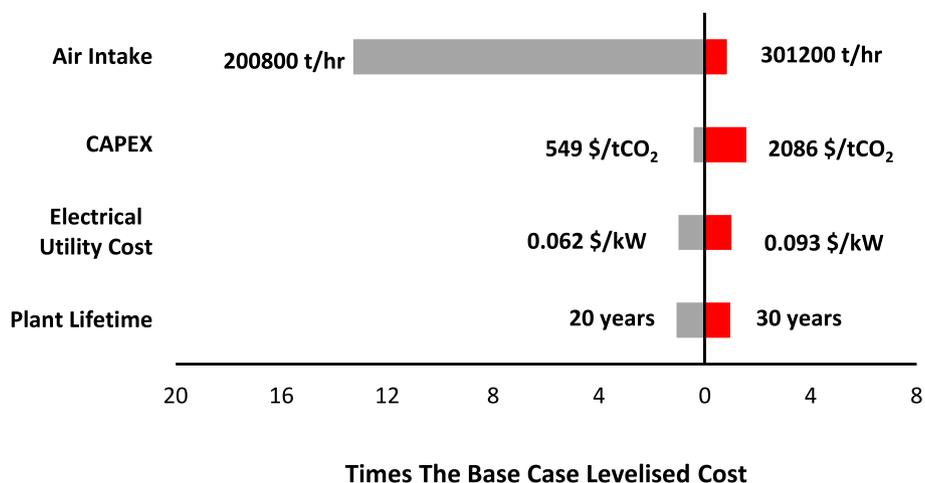


Fig. 7. Tornado plot of key system parameters and their effect on LCOD.

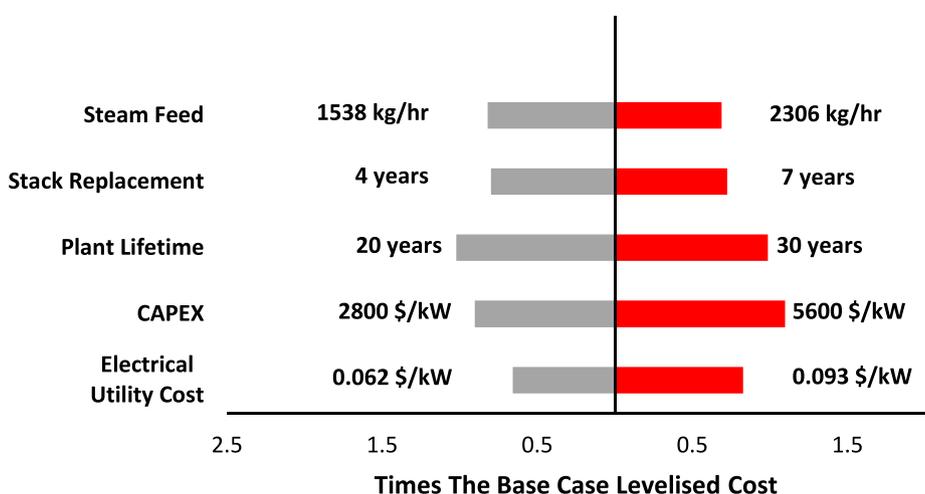


Fig. 8. Tornado plot of key system parameters and their effect on LCOH.

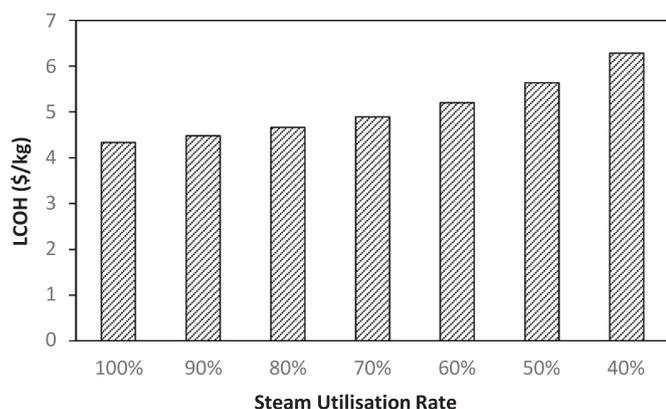


Fig. 9. Effect of steam utilisation rate on LCOH.

benchmark for analysis due to the detailed energy and cost breakdown of the plant modelled. It is also one of the few plants that has been constructed and functions at a large scale.

A comparison of levelised costs for CO₂ capture is presented in Table 5. The LCOD falls within the expected limits for liquid DAC methods. This appears to be further validated by the results published by Carbon Engineering which claim to have acquired a levelised cost of

Table 5 Comparison of LCOD across different technologies and sources [56].

Technology	Unit	Value
Point source: high CO₂ concentrations		
Natural Gas Processing	\$/tCO ₂	15–25
Ammonia	\$/tCO ₂	25–35
Hydrogen (Steam Methane Reforming)	\$/tCO ₂	50–80
Point source: low CO₂ concentrations		
Iron and steel	\$/tCO ₂	40–100
Power Generation	\$/tCO ₂	50–100
Cement	\$/tCO ₂	60–120
Non-point source: DAC methods		
HT-DACC	\$/tCO ₂	95–230
LT-DACC	\$/tCO ₂	100–600
Present system	\$/tCO ₂	124

carbon capture in the range of 94–232 \$/tCO₂ [17]. Point source carbon abatement costs are introduced to provide a wider context for current cost competitive technologies and applications. The majority of energy demand for the DAC system is required for heating purposes in the calciner and slaker. Additional heating in the calciner would be required from supplementary heater to bring the SMR steam temperature up from 800 °C to the required 900 °C. As the majority of thermal energy used is from waste heat and electrical utilities are assumed to be supplied directly by the reactor, it can be assumed that this would be “free” and

hence would not contribute to the cost of heating, hence the relatively low levelised cost reported.

It is worth noting that the CAPEX and various other costs associated with DACC are elusive and unreliable given the immature nature of the technology. The predominant factor that would influence the LCOD appears to be the air intake, as visualised in Fig. 7. Less air intake would increase system costs, particularly when considering that CO₂ makes up approximately 0.06% of atmospheric air by mass. Hence, it would be in the best interest to maximise the airflow in order to reduce costs. This could be achieved by utilising efficient fan components or placing the unit in a more carbon intense area, such as areas of high vehicular traffic or large, populous cities. This would be more achievable when powered by an SMR due to the smaller size and modular makeup of the plants. However, this does present issues - a carbon capture plant of this scale would take up significant land space, of which would influence decisions regarding suitable locations. Legal complications regarding planning permission could arise, yet the severity of this may be reduced given the magnitude of initiatives and funding being directed to support the R&D of this sector. Nevertheless, the estimated LCOD falls within the expected range of HT DACC technologies and is only 3% more costly than the most expensive point-source abatement method (cement). This presents a potential cost-competitive solution, particularly in the near-future as the technology matures.

The LCOH calculated from the simulated HTSE plant is compared with other hydrogen production methods as seen in Fig. 10. It is stated that the present system is the most costly method of hydrogen generation. However, these values are incredibly subjective, as mentioned previously, where various factors such as plant size, location, utility feed, and more can significantly alter the costs. For reference, despite the range of values highlighted in the aforementioned table, the simulation calculation is actually cheaper than the projected value estimated by the Department of Energy in the United States, which estimated an LCOH of 4.95 \$/kgH₂ in 2016 [57]. As it stands, the estimated LCOH from the simulation data does not propose a cost competitive solution when compared to more established methods.

Reasons for the deviation in economic calculations may arise from the scaling of the plant in order to facilitate its implementation alongside the thermal and electrical output of an SMR. In the reference setup of the HTSE plant, the output of hydrogen was set to be 50,000 kg/d and thus required a nuclear steam flow of 1921 kg/s or 6916 t/hr. Assuming that the heating of the HTSE plant were to be entirely satisfied by nuclear waste heat from generated steam, this plant setup would be deemed infeasible. Taking the thermal efficiency to be 36% as previously stated, this would yield about 740 MW of waste heat, of which has the capacity to vaporise water at around 817 t/hr which would not meet the requirement as stated in the reference simulation. However, if the

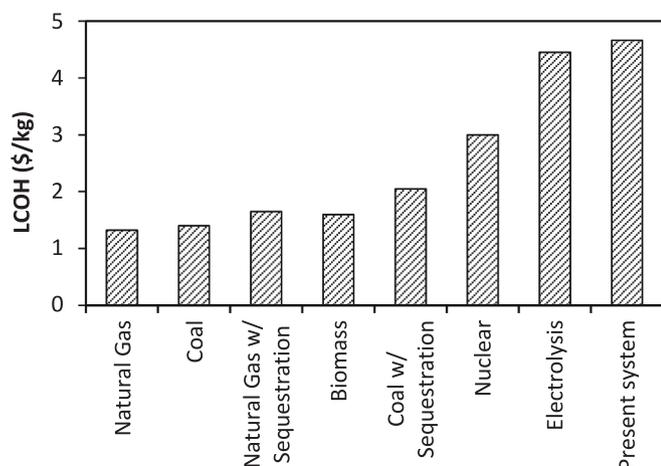


Fig. 10. Comparison of LCOH based on feedstock and method [58].

heating requirement were to be met in the triple-digit tonne range, the stack power demand would be the bottleneck to the HTSE operation as it would require around 250 MW. At this point, the solution does become cost competitive as the LCOH drops to around 2.00 \$/kgH₂ depending on increased hydrogen output. Generally, the power demands of the HTSE unit are predominantly electrical, at a ratio of 8:2 of electrical to thermal requirements, as verified in literature.

Additionally, the capacity factor of both simulations was set at 100% for simplicity. In reality and in most literature, the capacity factor is usually said to be around 90% to signify plant shutdowns and other operational requirements; these factors would influence the calculated levelised costs, where current estimations may be more optimistic [57]. As shown in the tornado plots, economic results can vary based on certain parameters. These can be further influenced by location, as mentioned previously. For example, global location would influence the utility costs of electricity and hence the overall value of levelised costs. This factor will be difficult to forecast in the European region due to political unrest and its impact of excessive, volatile energy prices, of which have increased by around 15 times 2021 rates [59]. This issue would be more weighted when considering the HTSE system given its larger reliance on electrical energy.

In order to meet expectations set out by the Paris Agreement, 7–10 GtCO₂ must be captured or used per year until 2050 [60]. To emulate this, projected LCOD can be modelled by implementing a learner curve for three given scenarios - conservative case where 50% of the target is satisfied, base case where 75% of the target is satisfied and net-zero case where the target is met. These scenarios correspond to learner rates of 15%, 12.5%, and 10%, respectively. Learner curve rates are in accordance with achieving the Paris Agreement goals of net-zero by 2050. The same cases are applied to the HTSE model for simplicity. Results are highlighted in Figs. 11 and 12.

Under the net-zero case, projected values for LCOD and LCOH could reach around 31 \$/tCO₂ and 1.16 \$/kgH₂ by 2050, respectively, which are within range of those stated in various publications from accredited energy institutions [60,61]. The projected values of these technologies cannot be reliably verified until the TRL of the systems is improved and more are built at a commercial scale. It is possible that rapid technological developments and rollout of certain credit schemes may further reduce future costs.

4.2. Implementation and market behaviour

The data gathered does indicate that both hydrogen production and DACC would be technically possible, particularly if the SMR were to be built with the sole purpose of powering these systems. There also presents opportunity to combine these two systems and the wholesale of nuclear electricity with the plant. This would be heavily dependent on grid demand and would vary from region to region, particularly when considering the magnitude of required electrical energy for the systems' operations. As the DACC system is more dependent on thermal energy, it

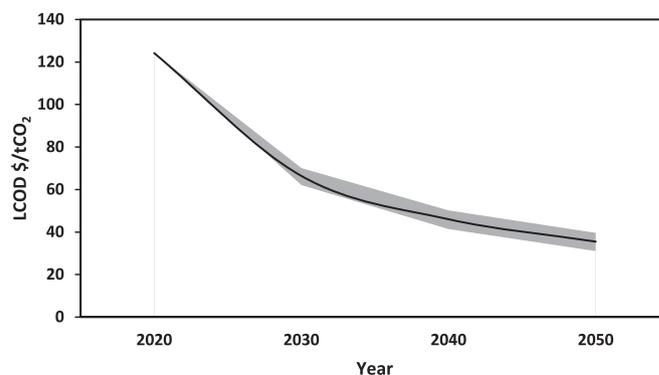


Fig. 11. Learner curve estimations of future LCOD.

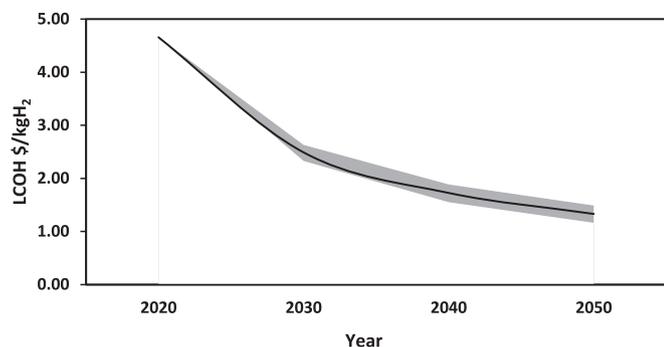


Fig. 12. Learner curve estimations of future LCOH.

may be more beneficial to power this by an SMR as an auxiliary process if the main aim were to deliver electricity to the grid. Alternatively, using an SMR to power both DACC and HTSE in standalone operations would be possible and may be more economical as opposed to a grid-hydrogen output due to the large electrical demands of HTSE and the smaller electrical outputs of SMRs when compared to mainstream nuclear power plants.

To gain a top-level view of profitability, an analysis into the NPV and Internal Rate of Return (IRR) of the following systems has been conducted: wholesale electricity and DACC; wholesale electricity and HTSE; wholesale electricity, DACC, and HTSE; standalone powering of DACC and HTSE. It is assumed that the products of such systems will entirely meet market demand and hence will be sold without any remainder product. The projected LCOE from SMRs varies due to the immaturity of the technology, however, assuming a ballpark average of 0.0775 \$/kWh and operation of 365 days a year, 24 h a day, yearly revenues can be expected to reach around \$203.67 million for a 300 MW plant. The parameters based on the aforementioned scenarios for estimating NPV and IRR are shown in Table 6, and the results of NPV and IRR are shown in Fig. 13.

From Fig. 13, it is implied that a combination of wholesale electricity and HTSE hydrogen production would be most profitable based solely upon the NPV and IRR calculated. This may be due to the high assumed sell price. However, it is unlikely that this would yield the reported revenues due to the above-market sell price of the hydrogen produced and hence current demand is likely to not be high enough to warrant such pricing. Further complications arise when considering grid demand. The hydrogen cash flow is based upon the output from the benchmark scenario previously modelled; this model does not sufficiently capitalise on the available electricity nor the steam flow of the SMR however these parameters are subject to grid demand, hence this would need to be accounted for to explore an optimised electrical generation to hydrogen output ratio. Therefore, this is not an accurate result.

Table 6
Financial parameters for estimating NPV and IRR.

Scenario	Unit	Cash flow from power	Cash flow from product	Total cash flow
Wholesale Electricity ¹ and DACC ²	m	201.26	58.88	260.14
Wholesale Electricity ¹ and HTSE ³	m	199.00	8.98	207.98
Wholesale Electricity ¹ , DACC ² , and HTSE ³	m	196.59	58.88 (DACC)	264.45
Standalone powering of DACC ² and HTSE ^{3*}	m	0	58.88 (DACC)	272.63
	\$/yr		213.75 (HTSE)	

¹ Price of wholesale electricity: 0.0775 \$/kWh.

² DACC CO₂ Carbon Credits: 60 t/CO₂.

³ HTSE Based Hydrogen: *1.75–5.12 \$/kgH₂.

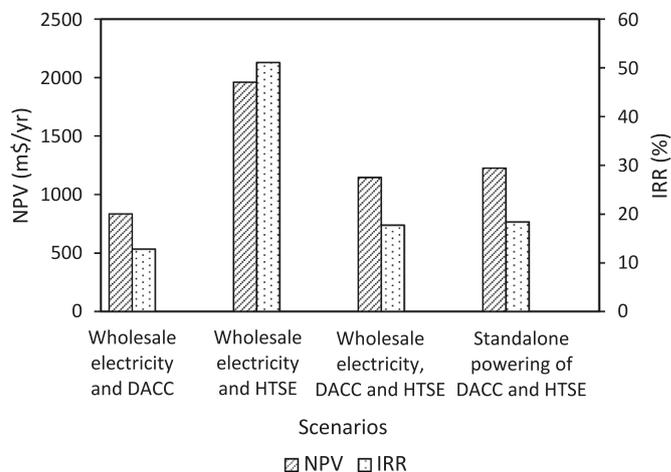


Fig. 13. Estimated NPV and IRR of various scenarios.

A more reasonable setup would be the standalone DACC and HTSE system, again based on the high NPV and large IRR. This setup allows for a reduced LCOH and hence proposes a competitive price for hydrogen production as the electrical output of the SMR can be maximised for the HTSE unit. In this analysis, the opportunity cost of selling the electricity was not considered as part of the OPEX, hence the reduced LCOH. Reasons for this is that the cost can be assumed to be recovered via the combination of carbon credits and hydrogen production and that the electricity production is done “in-house”.

To reiterate, cash flows of such systems are difficult to model. As with the unit costs, the estimated selling prices will be heavily influenced by geography, political motives, and funding opportunities. The market for such technologies is incredibly volatile yet shows promising development for reduced expenditures and increased revenues as demand for decarbonisation rises. These factors are facilitated by planned developments of various credit schemes, such as Carbon Credits (CCs) and Zero-Emission Credits (ZECs). The ZECs may play a significant role in promoting the profitability of SMR outputs by awarding SMR plants with compensation for the production of electricity without GHG emissions and possibly emission less hydrogen production [62]. This will also allow for some protection against market failure. On the contrary, certain regions may be imposing taxes on nuclear energy due to political debates which may hinder nuclear power plant profitability, as seen across various European regions such as Germany and Switzerland but it is likely this will be outweighed by the pressure to decarbonise the energy sector, of which nuclear power is an attractive option [63].

4.3. Future scope of work

The study offered a simplified setup of the combined systems in order to identify overarching trends of the plant. To further develop this research, a more detailed power delivery system should be modelled to account for any losses present in the transport of nuclear waste heat across the systems, particularly regarding the design specifications of heat exchangers — waste heat recovery was assumed to be 100% in this study and thus would not reflect the reality of heat transfer effectively. It is possible that energy recovery synergies between the technologies exist and so should be modelled to improve the overall efficiency of the integrated system. Furthermore, structural developments were not considered. In the case of incorporating these processes to SMRs, structural developments would need to be explored in order to verify the delivery and safety of such a setup.

A more in-depth HTSE simulation should be modelled to produce a tailored setup depending on SMR design specifications. CAPEX costs associated with HTSE units vary majorly depending on the stack voltage levels, power of the unit, current density, etc. These factors were outside

the scope of this study but their significance cannot be disregarded. Hence, a possible relationship between these factors and various SMR design specifications may exist and should be investigated to facilitate more efficient integration opportunities, improve hydrogen production rates, and reduce energy demands.

Furthermore, future SMR capacity is expected to improve. A general model of the SMR setup with high level calculations to identify general operating trends was used in this study. To expand on this research, more in depth heat transfer calculations should be conducted and SMR design makeup should be explored in order to effectively facilitate such energy transfers to its other processes. Investigations into the decoupling of the power island from the DACC and HTSE units should be investigated to identify the safest method of operation. The validity of economic projections will become more reliable as these technologies come to market fruition, which is expected in the next decade or so. Until then, year-on-year trends should be analysed and geographic influence should be investigated in more detail. The majority of sources used in this study for DACC technology in particular are biased towards Western geographies, mostly the USA. Location of DACC builds may have a large influence on levelised costs when taking into account region-specific funding, policies, and CO₂ content hence assessment into this factor would allow for identification of optimised areas for DACC construction. It is probable that this area will experience the greatest volatility in results because of the various factors that influence pricing and rapid technological developments in the sector, hence these trends should be closely followed.

5. Conclusion

This study proposed a functional theoretical model of a high temperature liquid sorbent direct air carbon capture plant in conjunction with a high temperature steam electrolysis unit, utilising the waste heat from a small modular reactor to assist in meeting thermal energy requirements of both systems. The major results are summarised below:

- DACC base case simulation results indicate an electricity and thermal demand of 31.67 kWh/tCO₂ and 126.33 kWh/tCO₂ respectively at a levelised cost of 124.15 \$/tCO₂.
- An electricity demand to hydrogen output of 34.37 kWh/kgH₂ and a thermal demand of 0.02 kWh/kgH₂ would result in a levelised cost of 4.66 \$/kgH₂.
- Both cases highlight how higher production rates would result in larger energy demands at a linear rate for hydrogen production and a similar relationship for DACC. Nevertheless, this would lower the levelised costs.

It is important to note that the estimated LCOD fell within the ranges reported in literature and does imply an affordable solution compared to similar setups. However, the cost of DACC is still much larger compared to point source abatement methods. Conversely, the LCOH calculated did not present the technology as cost-competitive as compared to more established methods. This is most likely due to the base case simulation parameters. In other words, further work that identifies an optimal steam flow rate by employing multi-objective optimisation techniques could result in more competitive costs. Nevertheless, the projected increase in demand with stricter climate policies would imply a reduction in levelised costs of both technologies and hence better cost-competitiveness as research and innovation advances. Due to differences in electrical and thermal demands, it may be more beneficial to integrate a continuous DACC system with an SMR if electrical energy were to be sold to the grid. Alternatively, a standalone HTSE-DACC system to be powered by an SMR would be more beneficial if wholesale electricity is not the intended output.

Further work should be conducted to optimise the energy synergies between the SMR and the DACC-HTSE systems. Due to the main limitation of this study i.e., the heavy reliance on secondary data from

various technical simulations and the nature of economic data extrapolation, the integrated system can be further investigated by employing detailed exergoeconomic and multi-objective optimisation methodologies, which may provide a better understanding of the integrated system's performance.

CRedit authorship contribution statement

Brittney Slavin: Writing – original draft, Software, Methodology, Investigation, Data curation, Conceptualization. **Ruiqi Wang:** Writing – review & editing, Software, Methodology, Investigation, Formal analysis. **Dibyendu Roy:** Writing – review & editing, Visualization, Methodology, Investigation, Formal analysis. **Janie Ling-Chin:** Writing – review & editing, Visualization, Supervision, Methodology, Conceptualization. **Anthony Paul Roskilly:** Supervision, Project administration, Funding acquisition.

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.

Acknowledgments

This research was delivered with financial support from the UK Research Council (UKRI) for a project entitled “Zero-Carbon Emission Integrated Cooling, Heating and Power (ICHPP) Networks” (EP/T022949/1).

References

- [1] Environmental Protection Agency. Climate change indicators: greenhouse gases. Environ Prot Agency; 2023. <https://www.epa.gov/climate-indicators/greenhouse-gases> (accessed July 4, 2023).
- [2] International Energy Agency. Defying expectations, CO₂ emissions from global fossil fuel combustion are set to grow in 2022 by only a fraction of last year's big increase. IEA; 2023. <https://www.iea.org/news/defying-expectations-co2-emissions-from-global-fossil-fuel-combustion-are-set-to-grow-in-2022-by-only-a-fraction-of-last-year-s-big-increase> (accessed July 4, 2023).
- [3] IEA. Greenhouse gas emissions from energy data explorer. IEA; 2021. <https://www.iea.org/data-and-statistics/data-tools/greenhouse-gas-emissions-from-energy-data-explorer> (accessed July 4, 2023).
- [4] British Geological Survey. Understanding carbon capture and storage. Br Geol Surv; 2023. <https://www.bgs.ac.uk/discovering-geology/climate-change/carbon-capture-and-storage/> (accessed July 4, 2023).
- [5] Restrepo-Valencia S, Walter A. BECCS opportunities in Brazil: comparison of pre and post-combustion capture in a typical sugarcane mill. Int J Greenh Gas Control 2023;124:103859. <https://doi.org/10.1016/j.ijggc.2023.103859>.
- [6] Kuru T, Khaleghi K, Livescu S. Solid sorbent direct air capture using geothermal energy resources (S-DAC-GT) – region specific analysis. Geoenery Sci Eng 2023; 224:211645. <https://doi.org/10.1016/j.geoen.2023.211645>.
- [7] Young J, McQueen N, Charalambous C, Foteinis S, Hawrot O, Ojeda M, et al. The cost of direct air capture and storage can be reduced via strategic deployment but is unlikely to fall below stated cost targets. One Earth 2023;6:899–917. <https://doi.org/10.1016/j.oneear.2023.06.004>.
- [8] Fasih M, Efimova O, Breyer C. Techno-economic assessment of CO₂ direct air capture plants. J Clean Prod 2019;224:957–80. <https://doi.org/10.1016/j.jclepro.2019.03.086>.
- [9] World Nuclear Association. Hydrogen production and uses. World Nucl Assoc; 2021. <https://world-nuclear.org/information-library/energy-and-the-environment/hydrogen-production-and-uses.aspx>.
- [10] International Energy Agency. Hydrogen supply. <https://www.iea.org/reports/hydrogen-supply>; 2022 (accessed March 1, 2023).
- [11] Fallah Vostakola M, Ozcan H, El-Emam RS, Amini Horri B. Recent advances in high-temperature steam electrolysis with solid oxide electrolyzers for green hydrogen production. Energies 2023;16. <https://doi.org/10.3390/en16083327>.
- [12] Shiva Kumar S, Himabindu V. Hydrogen production by PEM water electrolysis – a review. Mater Sci Energy Technol 2019;2:442–54. <https://doi.org/10.1016/j.mset.2019.03.002>.

- [13] World Nuclear Association. Small nuclear power reactors. World Nucl Assoc; 2023. <https://www.world-nuclear.org/information-library/nuclear-fuel-cycle/nuclear-power-reactors/small-nuclear-power-reactors.aspx>.
- [14] European Commission. Cogeneration of heat and power. Eur Commision; 2023. https://energy.ec.europa.eu/topics/energy-efficiency/cogeneration-heat-and-power_en.
- [15] International Energy Agency. Direct air capture. <https://www.iea.org/reports/direct-air-capture>; 2022 (accessed March 1, 2023).
- [16] International Energy Agency. Energy technology perspectives 2020 - Special report on carbon capture utilisation and storage: CCUS in clean energy transitions. 2020. <https://doi.org/10.1787/208b66f4-en>.
- [17] Keith DW, Holmes G, St. Angelo D, Heidel K. A process for capturing CO₂ from the atmosphere. *Joule* 2018;2:1573–94. <https://doi.org/10.1016/j.joule.2018.05.006>.
- [18] Carbon Engineering. Carbon engineering. <https://carbonengineering.com/our-technology/>; 2023 (accessed July 11, 2023).
- [19] Herzog H. Direct air capture: a process engineer's view (low-carbon energy center webinar). MIT Energy Initiat 2021. <https://www.youtube.com/watch?v=9uRHKnQ3b5s>.
- [20] Kiani A, Jiang K, Feron P. Techno-economic assessment for CO₂ capture from air using a conventional liquid-based absorption process. *Front Energy Res* 2020;8: 1–13. <https://doi.org/10.3389/fenrg.2020.00092>.
- [21] Terlouw T, Treyer K, Bauer C, Mazzotti M. Life cycle assessment of direct air carbon capture and storage with low-carbon energy sources. *Environ Sci Technol* 2021;55:11397–411. <https://doi.org/10.1021/acs.est.1c03263>.
- [22] Climeworks. Direct air capture: Our technology to capture CO₂. Climeworks; 2023. <https://climeworks.com/direct-air-capture> (accessed July 11, 2023).
- [23] Global Thermostat. The air carbon solution. Glob Thermostat; 2023. <https://www.globalthermostat.com/>.
- [24] McQueen N, Psarras P, Pilorgé H, Liguori S, He J, Yuan M, et al. Cost analysis of direct air capture and sequestration coupled to low-carbon thermal energy in the United States. *Environ Sci Technol* 2020;54:7542–51. <https://doi.org/10.1021/acs.est.0c00476>.
- [25] Slesinski D, Litzelman S. How low-carbon heat requirements for direct air capture of CO₂ can enable the expansion of firm low-carbon electricity generation resources. *Front Clim* 2021;3. <https://doi.org/10.3389/fclim.2021.728719>.
- [26] European Commission. Hydrogen. Eur Commission; 2023. https://energy.ec.europa.eu/topics/energy-systems-integration/hydrogen_en (accessed July 11, 2023).
- [27] Frazer-Nash Consultancy. Low carbon hydrogen supply 2 competition - stream 1 phase 1: Summaries of successful projects. <https://www.gov.uk/government/publications/low-carbon-hydrogen-supply-2-competition-successful-projects/low-carbon-hydrogen-supply-2-competition-stream-1-phase-1-summaries-of-successful-projects>; 2022.
- [28] Office of Energy Efficiency & Renewable Energy. Hydrogen production processes. US Dep ENERGY; 2023. <https://www.energy.gov/eere/fuelcells/hydrogen-production-processes>.
- [29] Jalili M, Ghazanfari Holagh S, Chitsaz A, Song J, Markides CN. Electrolyzer cell-methanation/Sabatier reactors integration for power-to-gas energy storage: thermo-economic analysis and multi-objective optimization. *Appl Energy* 2023; 329:120268. <https://doi.org/10.1016/j.apenergy.2022.120268>.
- [30] Nieminen J, Dincer I, Naterer G. Comparative performance analysis of PEM and solid oxide steam electrolyzers. *Int J Hydrogen Energy* 2010;35:10842–50. <https://doi.org/10.1016/j.ijhydene.2010.06.005>.
- [31] Ebbesen SD, Jensen SH, Hauch A, Mogensen MB. High temperature electrolysis in alkaline cells, solid proton conducting cells, and solid oxide cells. *Chem Rev* 2014; 114:10697–734. <https://doi.org/10.1021/cr5000865>.
- [32] Cui J, Aziz M. Techno-economic analysis of hydrogen transportation infrastructure using ammonia and methanol. *Int J Hydrogen Energy* 2023;48:15737–47. <https://doi.org/10.1016/j.ijhydene.2023.01.096>.
- [33] Hosseini SE. Design and analysis of renewable hydrogen production from biogas by integrating a gas turbine system and a solid oxide steam electrolyzer. *Energy Convers Manage* 2020;211:112760. <https://doi.org/10.1016/j.enconman.2020.112760>.
- [34] Assareh E, Mousavi Asl SS, Agarwal N, Ahmadijad M, Ghodrat M, Lee M. New optimized configuration for a hybrid PVT solar/electrolyzer/absorption chiller system utilizing the response surface method as a machine learning technique and multi-objective optimization. *Energy* 2023;281:128309. <https://doi.org/10.1016/j.energy.2023.128309>.
- [35] Wang Y, Chen H, Qiao S, Pan P, Xu G, Dong Y, et al. A novel methanol-electricity cogeneration system based on the integration of water electrolysis and plasma waste gasification. *Energy* 2023;267:126490. <https://doi.org/10.1016/j.energy.2022.126490>.
- [36] Locatelli G, Boarin S, Fiordaliso A, Ricotti ME. Load following of small modular reactors (SMR) by cogeneration of hydrogen: a techno-economic analysis. *Energy* 2018;148:494–505. <https://doi.org/10.1016/j.energy.2018.01.041>.
- [37] Coppiters D, De Paepe W, Contino F. Surrogate-assisted robust design optimization and global sensitivity analysis of a directly coupled photovoltaic-electrolyzer system under techno-economic uncertainty. *Appl Energy* 2019;248:310–20. <https://doi.org/10.1016/j.apenergy.2019.04.101>.
- [38] Bhandari R, Shah RR. Hydrogen as energy carrier: techno-economic assessment of decentralized hydrogen production in Germany. *Renew Energy* 2021;177:915–31. <https://doi.org/10.1016/j.renene.2021.05.149>.
- [39] Yilmaz C. Thermo-economic modeling and optimization of a hydrogen production system using geothermal energy. *Geothermics* 2017;65:32–43. <https://doi.org/10.1016/j.geothermics.2016.08.008>.
- [40] Bhattacharyya R, Misra A, Sandeep KC. Photovoltaic solar energy conversion for hydrogen production by alkaline water electrolysis: conceptual design and analysis. *Energy Convers Manage* 2017;133:1–13. <https://doi.org/10.1016/j.enconman.2016.11.057>.
- [41] Coppiters D, Costa A, Chauvy R, Dubois L, De Paepe W, Thomas D, et al. Energy, Exergy, Economic and Environmental (4E) analysis of integrated direct air capture and CO₂ methanation under uncertainty. *Fuel* 2023;344:127969. <https://doi.org/10.1016/j.fuel.2023.127969>.
- [42] Daniel T, Masini A, Milne C, Nourshagh N, Iranpour C, Xuan J. Techno-economic analysis of direct air carbon capture with CO₂ utilisation. *Carbon Capture Sci Technol* 2022;2:100025. <https://doi.org/10.1016/j.cst.2021.100025>.
- [43] Tomberg M, Heddrich MP, Ansar SA, Friedrich KA. Operation strategies for a flexible megawatt scale electrolysis system for synthesis gas and hydrogen production with direct air capture of carbon dioxide. *Sustain Energy Fuels* 2022;7: 471–84. <https://doi.org/10.1039/d2se01473d>.
- [44] Ishaq H, Crawford C. CO₂-based alternative fuel production to support development of CO₂ capture, utilization and storage. *Fuel* 2023;331:125684. <https://doi.org/10.1016/j.fuel.2022.125684>.
- [45] Ji Y, Yong JY, Liu W, Zhang XJ, Jiang L. Thermodynamic analysis on direct air capture for building air condition system: balance between adsorbent and refrigerant. *Energy Built Environ* 2022;4:399–407. <https://doi.org/10.1016/j.enbenv.2022.02.009>.
- [46] Cheng P, Thierry DM, Hendrix H, Dombrowski KD, Sachde DJ, Realf MJ, et al. Modeling and optimization of carbon-negative NGCC plant enabled by modular direct air capture. *Appl Energy* 2023;341:121076. <https://doi.org/10.1016/j.apenergy.2023.121076>.
- [47] Cole GM, Greene JM, Quinn JC, McDaniel B, Kemp L, Simmons D, et al. Integrated techno-economic and life cycle assessment of a novel algae-based coating for direct air carbon capture and sequestration. *J CO₂ Util* 2023;69:102421. <https://doi.org/10.1016/j.jcou.2023.102421>.
- [48] Liu W, Lin YC, Ji Y, Yong JY, Zhang XJ, Jiang L. Thermodynamic study on two adsorption working cycles for direct air capture. *Appl Therm Eng* 2022:214. <https://doi.org/10.1016/j.applthermaleng.2022.118920>.
- [49] Drechsler C, Agar DW. Intensified integrated direct air capture - power-to-gas process based on H₂O and CO₂ from ambient air. *Appl Energy* 2020;273:115076. <https://doi.org/10.1016/j.apenergy.2020.115076>.
- [50] Bianchi S. Process modelling of a Direct Air Capture (DAC) system based on the Kraft process. *POLITECNICO DI TORINO*; 2018.
- [51] Im-orb K, Visitdumrongkul N, Saebea D, Patcharavorachot Y, Arpornwichanop A. Flow-sheet-based model and exergy analysis of solid oxide electrolysis cells for clean hydrogen production. *J Clean Prod* 2018;170:1–13. <https://doi.org/10.1016/j.jclepro.2017.09.127>.
- [52] Frick K, Wendt D, Talbot P, Rabiti C, Boardman R. Techno-economic assessment of hydrogen cogeneration via high temperature steam electrolysis with a light-water reactor. *Appl Energy* 2022;306:118044. <https://doi.org/10.1016/j.apenergy.2021.118044>.
- [53] Wendt D, Knighton L, Boardman R. High temperature steam electrolysis process performance and cost estimates. 2022.
- [54] Hosseini J, Sadeghi M, Chitsaz A, Ranjbar F, Rosen MA. Exergy assessment and optimization of a cogeneration system based on a solid oxide fuel cell integrated with a Stirling engine. *Energy Convers Manage* 2017;143:448–58. <https://doi.org/10.1016/j.enconman.2017.04.021>.
- [55] Bermudez Jose, Evangelopoulou Stavroula, Pavan F. Electrolysers. <https://www.iea.org/reports/electrolysers>; 2022.
- [56] IEA. CCUS in clean energy transitions. <https://www.iea.org/reports/ccus-in-clean-energy-transitions>; 2020 (accessed March 1, 2023).
- [57] DOE. Hydrogen production cost from solid oxide electrolysis. https://www.hydrogen.energy.gov/pdfs/16014_h2_production_cost_solid_oxide_electrolysis.pdf; 2016 (accessed August 2, 2023).
- [58] NREL. Analyzing the levelized cost of centralized and distributed hydrogen production using the H₂A production model, version 2. <https://www.nrel.gov/docs/fy09osti/46267.pdf>; 2009 (accessed March 1, 2023).
- [59] Zettelmeyer Jeromin, Tagliapietra Simone, Zachmann Georg, Heussaff C. Beating the european energy crisis. IMF; 2022. <https://www.imf.org/en/Publications/fandd/issues/2022/12/beating-the-european-energy-crisis-Zettelmeyer> (accessed July 11, 2023).
- [60] Energy Transitions Commission (ETC). Carbon capture, utilisation and storage in the energy transition: Vital but limited. <https://www.energy-transitions.org/publications/carbon-capture-use-storage-vital-but-limited/>; 2022 (accessed August 2, 2023).
- [61] IEA. Direct Air Capture, A key technology for net zero. https://iea.blob.core.windows.net/assets/78633715-15c0-44e1-81df-41123c556d57/DirectAirCapture_Akeytechnologyfornetzero.pdf; 2022 (accessed March 1, 2023).
- [62] NEL. Zero-emission credits. <https://www.nel.org/corporatesite/media/filefolder/resources/reports-and-briefs/zero-emission-credits-201804.pdf>; 2018 (accessed March 1, 2023).
- [63] WNA. Economics of nuclear power. World Nucl Assoc; 2022. <https://world-nuclear.org/information-library/economic-aspects/economics-of-nuclear-power.aspx> (accessed July 11, 2023).