Research paper

AI-Based Modelling and Processing Technologies for Hydrogen Creation

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Abstract

This research aims to thoroughly analyse recent advancements in method demonstration and the implementation of Artificial Intelligence (AI) in integrated hydrogen production and carbon capture. The primary objective is to offer a detailed account of the anticipated role of AI in shaping future research endeavours related to blue hydrogen production and carbon capture. This involves a focus on Machine Learning (ML) applications in material development and process optimisation. The research provides an overview of AI and cycle demonstration in a relevant context, accompanied by a concise examination of recent developments in blue hydrogen production. The foundational instruments of AI modelling and processing are briefly outlined, and their application in blue hydrogen creation is discussed, considering both advantages and drawbacks. Ultimately, the research aims to deliver a comprehensive overview of the advancements in ML, emphasising its substantial contribution to accelerating blue hydrogen generation, particularly in the realms of material and process development. AI modelling and processing technologies are preferred for hydrogen creation due to their superior ability to optimise complex, data-intensive processes and accelerate material innovation, overcoming the limitations of traditional modelling methods.

Keywords: Artificial Intelligence · Machine Learning · Blue Hydrogen · Carbon Capture and Storage (CCS) · Steam Methane Reforming · Process Optimisation · Catalyst Discovery · Digital Twin Technology

1. INTRODUCTION

Machine Learning (ML) has emerged as a powerful tool across various industries, including compound design, but its application in this field remains fragmented (Saheb et al., 2022). Recent advancements in artificial intelligence, driven by cost-effective computing power and user-friendly programming environments (Lian et al., 2023; Magazzino et al., 2022), have facilitated significant progress. However, further research, particularly in areas such as consolidated sorbent catalyst material (CSCM), is essential to enhance interaction and optimise innovative cycle designs like sorbent-enhanced steam methane reforming (SE-SMR).

One notable trend is the utilisation of ML to improve adsorption cycles, such as pressure swing adsorption (PSA), commonly used in hydrogen production for high-purity H_2 output (Seto et al., 2016). Traditional methods for modelling such cycles have been found to be slow and less effective compared to ML-based approaches (Niyas & Thiyagarajan, 2023).

Hydrogen production is not only pivotal for decarbonising industrial processes but also plays a vital role in energy storage systems, particularly in integrating renewable energy sources into the grid. As a chemical energy carrier, hydrogen enables long-duration energy storage, complementing battery technologies in stabilising power systems and supporting ancillary services. This dual role makes blue hydrogen a critical component of future low-carbon energy systems. Recent works such as Gulraiz et al. (2025) and Amir et al. (2023) emphasise the strategic integration of hydrogen and battery storage for flexible and resilient energy infrastructure. By considering AI applications across production and system-level deployment, this study contributes to shaping hydrogen's role in the broader energy transition landscape.

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The convergence of ML, the Internet of Things (IoT), and robotics, under the umbrella of Industry 4.0, is reshaping synthetic design, particularly in hydrogen production (Zhang et al., 2023). This is crucial for achieving decarbonisation goals, with blue hydrogen playing a significant role in the transition to a low-carbon economy, alongside green hydrogen (Saheb et al., 2022). ML can expedite the adoption of low-carbon technologies by offering intelligent pathways for enhancing hydrogen production efficiency while ensuring high purity and low costs.

The complexity of traditional hydrogen production processes, such as blue hydrogen generation involving SMR and carbon capture, presents significant challenges related to efficiency, optimisation, and material development. Conventional modelling techniques often fall short in addressing these challenges due to their limited ability to handle intricate interactions among numerous process variables effectively. AI modelling and processing technologies are preferred because they offer advanced capabilities in analysing large datasets, optimising complex multi-variable systems, and accelerating the discovery and development of innovative materials (Magazzino, 2024). Thus, AI presents a promising solution to overcoming the limitations of traditional methods, significantly enhancing efficiency, cost-effectiveness, and sustainability in hydrogen production.

Despite recent studies focusing on blue hydrogen production and material design using AI (Lombardo et al., 2022), comprehensive specialist examinations of AI in blue hydrogen production are lacking. This review aims to fill this gap by providing an in-depth analysis of ML applications in hydrogen production processes, highlighting their potential to address limitations in traditional modelling methods and integrate with digital twin technology.

The scope of this paper encompasses a comprehensive evaluation of AI applications, particularly ML, in the development and optimisation of blue hydrogen production systems. By analysing recent advancements in AI-driven process modelling, catalyst and sorbent discovery, and system-level optimisation, this study aims to bridge the existing knowledge gap between traditional modelling techniques and emerging intelligent technologies. Thus, the potential of this research lies in its ability to inform future innovation in low-carbon hydrogen technologies, accelerate industrial adoption of digital twin systems, and support policy decisions through enhanced predictive modelling and operational efficiency. Table 1 offers a comparison between this research and related studies in the literature.

Table 1. Summary of Related Works

Reference	**Contribution**	**Limitation**	**How this study addresses it**
Guo et al. (2021)	Demonstrated energy-efficient SE-SMR using ML for reactor modelling	Focused on unit-level process modelling without material integration	Integrating catalyst/sorbent discovery and process modelling using AI
Namoun et al. (2022)	Applied ANN-GA hybrid optimisation for PSA units	Limited to a narrow range of operating variables and unit-specific optimisation	Extending modelling across multiple process stages, including reformers and CCS
How et al. (2020)	Eight-step PSA optimisation using ML and MATLAB	High computational time, lack of system-level analysis	Emphasising reduced training time with AI surrogates and full-cycle optimisation
Krogh (2008)	Developed ANN models for hydrogen purity and CO_2 capture optimisation	Did not explore digital twin integration or real-time prediction	Incorporating digital twin potential and predictive modelling in plant-scale design
Kabir et al. (2023)	ML-assisted catalyst discovery via DFT	Focuses mainly on materials without process linkage	Bridging material discovery with process integration for blue hydrogen
Lombardo et al. (2022)	General AI application in energy materials	No specific focus on hydrogen or CO_2 capture	Focusing on hydrogen-specific applications of AI in both materials and process optimisation

The remainder of this paper is structured as follows: Section 2 provides an overview of blue hydrogen processes; Section 3 discusses traditional modelling approaches for blue hydrogen production; Section 4 presents a technical overview and the utilisation of ML; Section 5 outlines the significant prospects of blue hydrogen generation using ML; and finally, Section 6 concludes with policy recommendations.

2. BLUE HYDROGEN PRODUCTION

This section provides a comprehensive overview of blue hydrogen production tactics, including CO_2 capture approaches, and a summary of the sorbents and impetuses used in this process. Yan and Haroon (2023) and Wu et al. (2024) comprehensively evaluate blue hydrogen creation.

2.1 Overview of Blue Hydrogen Processes

Blue hydrogen is a form of hydrogen produced from natural gas using carbon capture and storage (CCS) technology, aimed at reducing the environmental impact compared to traditional methods. Here's how it works: Natural gas undergoes a reaction with steam in a high-temperature reactor, yielding hydrogen, CO_2, and other byproducts. The CO-rich gas resulting from SMR is further processed to convert more CO into CO_2. The flue gas produced in this process is then subjected to a capture unit where CO_2 is separated using technologies such as amine scrubbing or membrane separation. The captured CO_2 is compressed into a liquid state and transported via pipelines or ships to be permanently stored in geological formations like depleted oil and gas reservoirs or saline aquifers.

Blue hydrogen technology is well-established, offering high hydrogen yields but also emitting significant CO_2. It provides several methods for capturing CO_2: capturing it before SMR, which offers high capture rates but requires complex integration; capturing it after SMR, which is simpler to integrate but has lower capture rates; or using pure oxygen instead of air in SMR, resulting in a concentrated CO_2 stream for easier capture.

Compared to traditional hydrogen production methods, blue hydrogen significantly reduces CO_2 emissions through CCS. It can leverage existing natural gas infrastructure and expertise, enabling faster deployment and potentially being more cost-competitive than other low-carbon hydrogen options like green hydrogen in the short term.

However, it's essential to acknowledge the limitations of blue hydrogen and ongoing efforts to improve capture rates and ensure safe and permanent CO_2 storage. The transition from traditional "dark" hydrogen production, which emits significant CO_2, to blue hydrogen creation is facilitated by advancements in carbon capture technologies, ensuring that CO_2 emissions are captured and stored effectively.

In the standard SMR process, desulfurised natural gas and steam are compressed and heated to 650 °C before entering the reformer, where reactions R1, R2, and R3 take place. Since these reactions are endothermic, heat or energy must be supplied to the reformer. The water-gas shift (WGS) reactor then facilitates further reactions, converting the resulting syngas into hydrogen. Figure 1 depicts the standard SMR procedure that does not include a carbon trap. The overall reaction during this SMR cycle is seen in R3.

$$left-rightCH_{4(g)} + H_2O_{(g)} \leftrightarrow CO_{(g)} + 3H_{2(g)} \Delta H_{298K} = 206.2 kJ.mol^{-1} \quad R1$$

$$suitableCO_{(g)} + H_2O_{(g)} \leftrightarrow CO_{2(g)} + H_{2(g)} \Delta H_{298K} = -41.2 kJ.mol^{-1} \quad R2$$

$$suitableCH_{4(g)} + 2H_2O_{(g)} \leftrightarrow CO_{2(g)} + 4H_{2(g)} \Delta H_{298K} = 165.2 kJ.mol^{-1} \quad R3$$

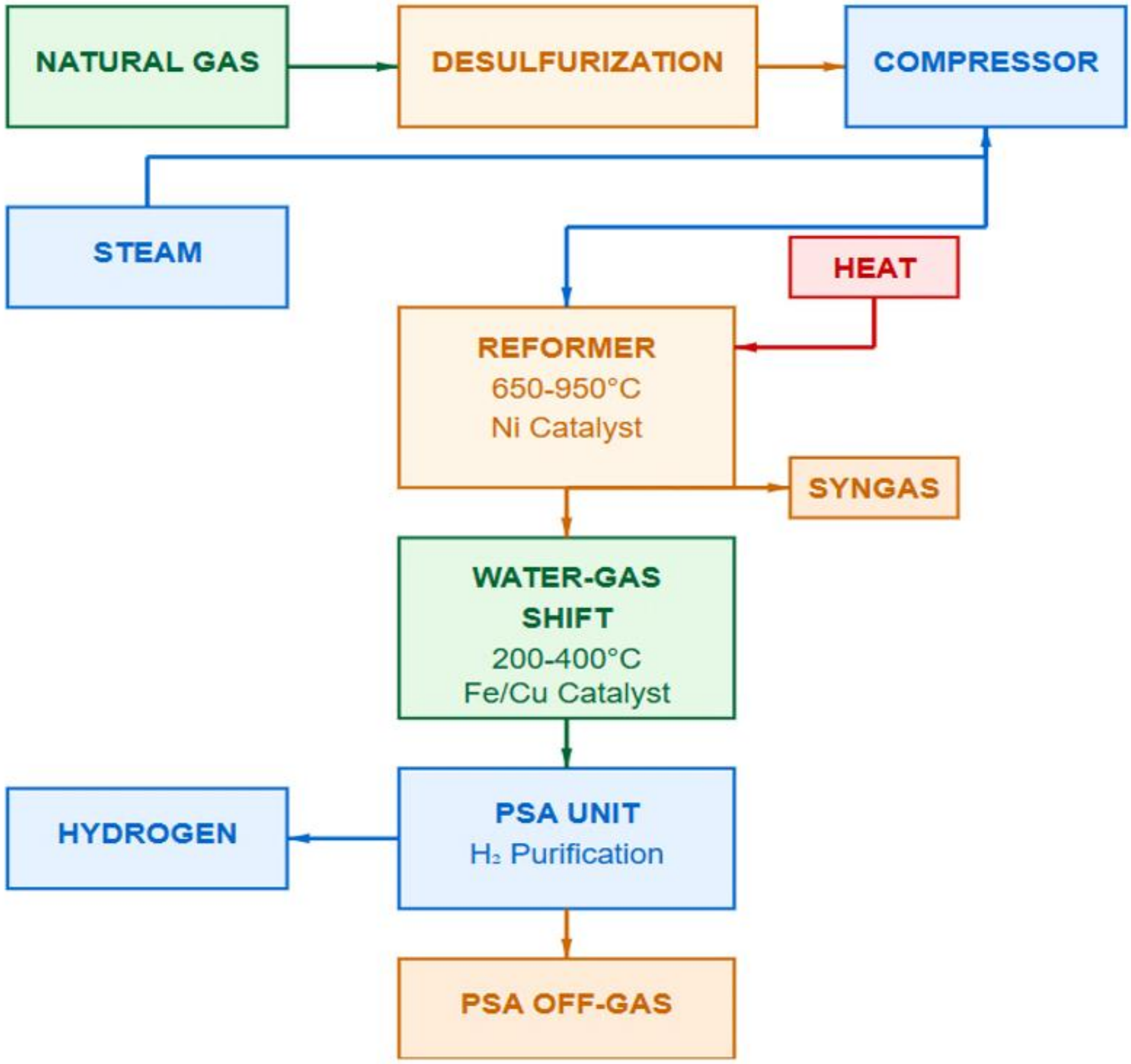

Figure 1. Process Flow Diagram for Steam Biogas Reforming, Simplified

2.1.1 Steam-Methane Conversion with Carbon Capture

While the traditional method of utilising amine scrubbing before PSA for CO_2 capture in hydrogen production has been prevalent, recent advancements present intriguing alternatives and considerations. Here is a closer look with additional information and details.

Amine solvents are used to chemically capture CO_2 from the SMR syngas, resulting in separate CO_2-rich and H_2-rich streams. The H_2-rich stream then undergoes PSA, where remaining trace impurities like CO, CO_2, and moisture are physically separated via selective adsorption on solid materials, yielding high-purity hydrogen.

Alternatively, CO_2 capture can occur before SMR using technologies like oxy-fuel combustion or membrane separation, resulting in a purer H_2 feed for PSA. While this approach may offer higher capture rates, it necessitates complex process integration.

Membranes can also selectively permeate CO_2 from the post-SMR syngas, offering advantages such as lower energy consumption but potentially lower capture rates compared to amine scrubbing.

Combining pre- and post-combustion capture methods can achieve higher overall capture rates, albeit with increased complexity and cost. Adsorption processes in PSA generally require less energy for sorbent regeneration compared to amine solvent regeneration in scrubbing. Furthermore, pre-combustion capture and certain membrane designs hold promise for achieving higher CO_2 capture percentages.

Post-combustion capture with membranes can be retrofitted into existing SMR facilities more easily than pre-combustion options. However, some alternative approaches, like pre-combustion capture and advanced membranes, are less mature than amine scrubbing and require further development and cost reduction.

It is essential to optimise the balance between the desired CO_2 capture percentage and economic feasibility. Additionally, different downstream applications may have varying purity requirements for hydrogen, which can influence the choice of CO_2 capture method. Conventional wisdom is that the first step in separating CO_2 from H_2 is to use amine scouring to remove the gas and then to send the H_2 stream that is free of CO_2 to a hydrogen filter (Figure 2).

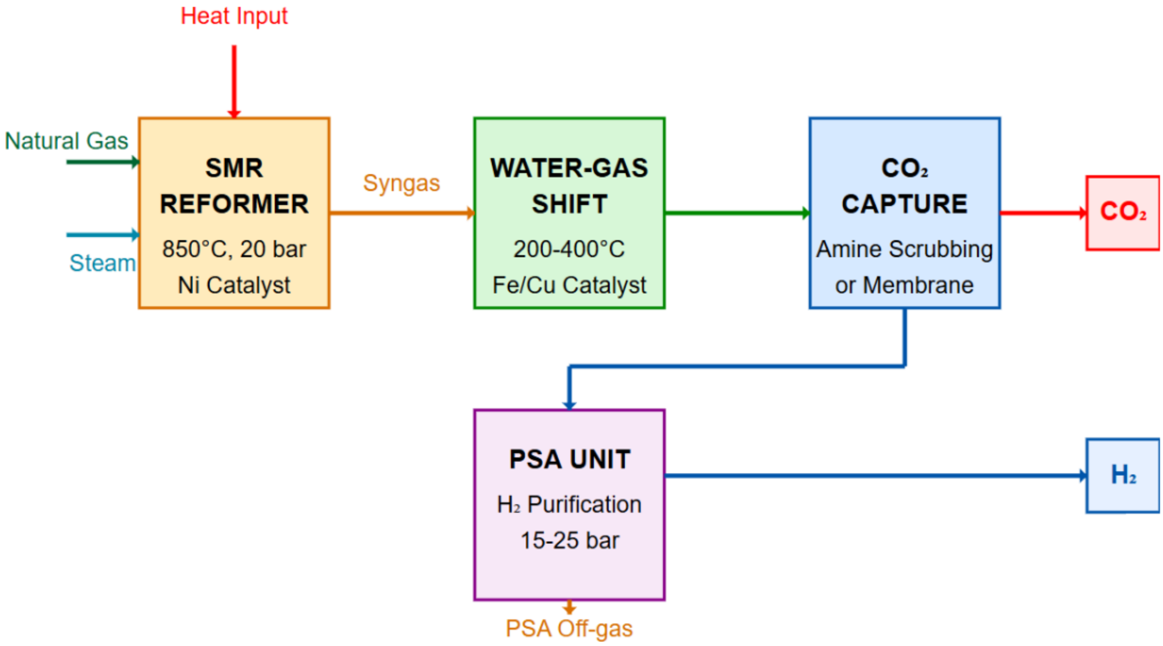

Figure 2. Process Flow-Sheet of SMR Process with Carbon Capture

Increases in CAPEX and OPEX inevitably result from adding more separation stages to the process. Much effort has gone into reducing costs via technical breakthroughs, creating inexpensive catalyst materials (Fang et al., 2023), and analysing the progression thermodynamically to ensure optimised heat mixing (Chen et al., 2023). Policy intervention in the form of financial incentives to decrease CO_2 emissions is an alternate strategy for cost reduction. Adopting such strategies worldwide has lowered the cost of renewable and low-carbon technology.

2.1.2 Improving Steam Methane Reforming via Sorption

The integration of carbon capture into the SMR cycle is enhanced by SE-SMR. This approach involves increasing the interaction within the cycle by incorporating the sorbent, typically calcium oxide (CaO), directly into the reformer instead of using it as a standalone unit. SE-SMR eliminates the need for WGS reactors and offers an alternative interaction design to improve efficiency.

Two essential cycle improvements are considered when integrating the sorbent into the reformer:

A. The reformer's internal CO_2 emissions occur simultaneously with its production, as highlighted in a study by Su et al. (2022). This imbalance necessitates additional hydrogen input to achieve further process optimisation.

B. The carbonisation of CaO is an exothermic process, as noted in research by Chen et al. (2023) and Haroon (2024), which reduces the reaction temperature and steam requirements for coke deposition on the catalyst (R4).

In essence, SE-SMR offers a promising approach to optimising hydrogen production processes by maximising interaction efficiency and addressing CO_2 emissions within the reforming cycle.

$$left - rightCaO_{(s)} + CO_{2(g)} \leftrightarrow CaCO_{3(s)}\Delta H_{298K} = -178.8\mathrm{kJ.mol}^{-}1 \qquad R4$$

Due to the exothermic response and intensification of the higher H_2 age via WGS reactions caused by utilizing calcium oxide as the sorbent, an extra WGS reactor is unnecessary (Guo et al., 2021). Researchers have looked at other sorbents because of problems with CaO's cyclability and deactivation after several rounds (Ghanbari et al., 2021).

2.1.3 Self-heating reforming

Recent research and development have led to the development of a more efficient and cost-effective method for producing blue hydrogen. Table 2 highlights the latest advancements in low-carbon hydrogen production, summarising new products, advancements in process optimisation aimed at reducing both capital and operational expenses of traditional methods, improvements in thermodynamic efficiency, and efforts to streamline the process to achieve higher CO_2 capture ratios. Some of these initiatives are discussed in Chen et al. (2023) and Haroon (2024).

Table 2. New Approaches for Low-Carbon Hydrogen Generation

Process	Process Synopsis
Increased absorption steam methane reforming with chemical looping combustion (SE-SMR + CLC)	If a chemical looping combustion unit is used instead of a traditional combustor, it is possible to store CO_2 of a high purity level without modifying the combustor. In the literature, many oxygen carriers have been described.
Chemical-looping reforming with sorption enhancement (SE-CLR)	This method uses a single reactor to improve and reduce methane. By replacing air with a solid oxygen carrier, an innovation in fuel combustion called CLR eliminates the need for collection technology while still creating high-purity CO_2.
Improved sorption steam methane gasification, often known as SE-SMG	We present a gasification reactor that gasifies biomass at high temperatures to create syngas and methane. After that, it's fed into the reformer to make hydrogen gas. There are no emissions when biomass is used as a precursor; nevertheless, gasification has a significant energy penalty.
SA-SMR, or solar-assisted steam methane reforming	The SMR method, which heats the molten salt using solar power, incorporates the pre-reformer; the use of solar heat generates minimal carbon dioxide emissions.

The primary focus of cycle development has been on incorporating sorbent material into the reactor for simultaneous CO_2 capture and H_2 production, as outlined in Table 1. Additionally, methods for reducing CO_2 emissions have been explored through the integration of solar electricity with low-carbon heat sources like chemical looping combustion (CLC). Efforts have also aimed at combining alternative feedstocks, such as SE-SMR, to mitigate the influence of methane as an ozone-depleting agent (Lombardo et al., 2022). Standard cycle modelling has played a crucial role in developing low-carbon H_2 solutions to assess the feasibility of these innovations at a reduced cost. Integrating innovations like CLC into the cycle provides a means for lower-carbon heat, reduces energy consumption compared to traditional CO_2 capture methods like amine scrubbing, and contributes to a decrease in CO_2 emissions (Nepal et al., 2021).

One aspect of standard cycle modelling involves simulating interactions under typical conditions, including mass transfer and intensity, to evaluate the outcomes of these interactions. Section 4 will delve into the latest developments in H_2 production and standard cycle modelling.

Recently, a novel cycle modelling approach has emerged, integrating ML into the process of showcasing hydrogen production. This comprehensive cycle optimisation involves developing ML surrogate models of H_2 generation by differentiating key operating parameters and key performance indicators (KPIs). The same principle applies to specific unit operations, such as a PSA unit (Osei et al., 2024). Faster simulation is achieved by selecting critical operating boundaries and reducing the model's complexity. The unique demonstration of these cycles enables accelerated simulation, which enhances process control and continuously provides insights into H_2 production processes. Section 6 provides a deeper exploration of ML's role in demonstrating hydrogen production progressions.

2.2 Research and Development of Blue Hydrogen Fuel

Research into blue hydrogen production has primarily focused on developing catalysts for efficient WGS reactions in reformer vessels, as depicted in Figure 3, and components for making blue hydrogen are presented in Table 3. While nickel-based catalysts are commonly used in standard SMR reactors, issues such as sintering at high temperatures can arise within these devices (Su et al., 22). Copper is another widely used catalyst in high-temperature WGS reactors, albeit it tends to be expensive (Hosseini and Wahid, 2016). However, recent efforts have shifted towards the development of CSCM for SE-SMR processes (John et al., 2022).

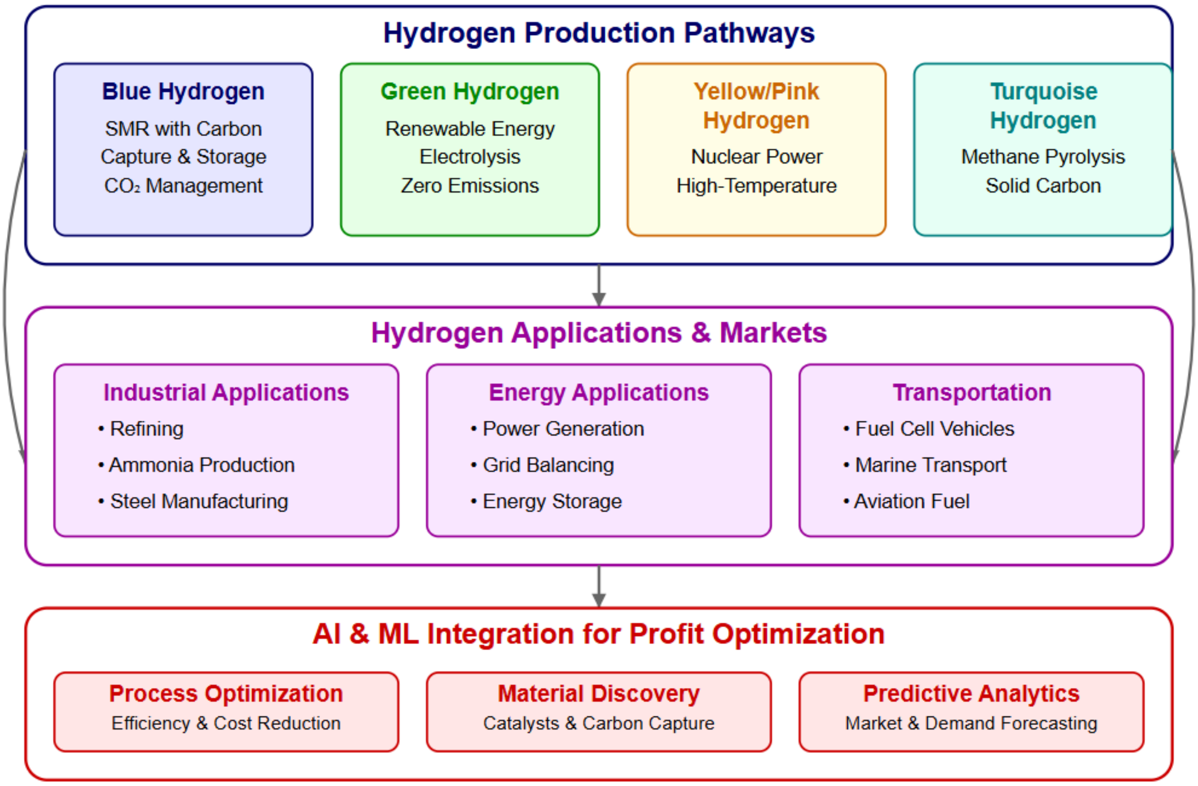

Figure 3. Profiting from the Fuel in the Future

Table 3. Ingredients for Making Blue Hydrogen

Molecule	Catalyst	Reaction	Overview
Ni-based Catalyst	Catalyst	SMR	They are less expensive than noble metals and are often used for SMR Metal oxide catalyst support ($Ni/MgAl_2O_4$), developed to lessen toxicity and improve conversion efficiency.
Single Atom Alloy (SAA)	Catalyst	WGS	SAA is an efficient and economical way to employ noble-metal catalysts while reducing the amount of metal used.
CaO	Sorbent	Adsorption	Because of its high CO_2 capture rate and cheap CaO cost, a significant concern is the gradual decrease in CO_2 sorption capacity over many cycles due to CaO sintering.
Ni/CaO–$Ca_5Al_6O_{14}$	Catalyst/Sorbent	SE-SMR	High stability and CaO utilisation are observed in the bi-functional catalyst stabilised with Ni/$Ca_5Al_6O_{14}$.
Hydrotalcite (HTC)	Sorbent	SE-SMR	Its enormous surface area and distinctive layered structure make it an alternative to CaO. But compared to other sorbents, it has a much-reduced sorption capacity.
Lithium orthosilicate (LTZ)	Sorbent	SE-SMR	Additionally, it possesses a lower temperature at which the regenerating process occurs, specifically around 700 °C. Nevertheless, the hydrogen manufacturing process is hindered by the joint influence of limited ability to absorb and sluggish decomposition frequency.

Techniques such as density functional theory (DFT) can provide insights into how new materials interact with CO_2 particles or their affinity with CH_4 in the hydrogen productivity process. ML has been found to be useful in the creation of new resources, namely in the evaluation of catalytic and absorbing substances, utilising quantitative structure-activity relationship (QSAR) methods. Metal-organic frameworks (MOFs) and other CO_2

capture materials have benefited from this (Zhdaneev and Frolov, 2024; Kanrar and Sarkar, 2024). Advancements in QSAR offer a framework for screening and ranking large compound libraries using key performance indicators (the material's activity), unlike traditional material screening methods that rely on experimental trial and error. Section 6 provides further elaboration on this topic.

3. BLUE HYDROGEN TRADITIONAL PROCESS MODELLING

It is critical for ensuring a large CO_2 capture rate and good H_2 purity. Direct contact demonstration and subsequent recreation are essential for an improved cycle for less-carbon hydrogen output. Around consumes much exploration zeroed in on process demonstrating, re-enactment, and enhancement of less-carbon hydrogen creation processes (Lakhouit et al., 2023).

Commonplace communication displaying code, such as Aspen, displaying the framework's physical and substance characteristics for the attention of unit administrators, modelling synthetic cycles, and gPROMS are also part of the process. Much research in the last decade has focused on improving and demonstrating these blue hydrogen output approaches (Li et al., 2020). Numerous demonstration projects have contributed to the enhancement of blue hydrogen processes. A semi-focused scale SE-SMR process was developed, capable of daily hydrogen delivery of 48 tons. Relative to conventional SMR, the simulation demonstrated an 82% improvement in energy efficiency and a 12% decrease in the cost of hydrogen production (Guo et al., 2021). The gulf temperature of the foaming fluidised couch remains the utmost significant variable because it has a substantial impact on the output ratio, CO_2 seizure, cost, and energy proficiency, according to a responsiveness analysis of the main working factors (temperature, tension, speed, and S/C proportion) upon process execution.

Examining SE-SMR elective cycle designs significantly determines the optimal interaction arrangement, confirming a more excellent CO_2 seizure ratio and good H_2 transparency. A thermodynamic analysis was conducted on these cycles concerning five critical execution metrics: Cold Gas productivity, Net proficiency, CH_4 transformation, H_2 transparency, and CO_2 capture. With an activist infection of 600 °C, a burden of 25 bar, and an S/C ratio of 5, case 4 (SE-SMR + public service announcement + CLC) was determined to be the optimal interaction design for a more significant CO_2 more excellent ratio (100 percent) and great H_2 virtue (100 percent) according to a responsiveness evaluation. These validate low TRL innovations, such as SE-SMR and CLC, to produce less-carbon hydrogen gas.

Awareness testing and other improvement methods may be illuminating when it comes to improving your handling skills. To accomplish better presentation, trend-designated important recital pointers (KPIs) will likely have a detailed understanding of the cycle and recognise the critical working limits that need to be simplified utilising the first standard displays. However, remember that regular improvement approaches, such as responsiveness research, often use an each-figure turn (OFAT) method. Although this method may help delineate personal work boundaries, it needs to reveal how they interact; this aspect may need more investigation. According to (Haixiang et al., 2017), a former study was focused on the plan of examination (DoE) approach, which goals to enhance by equally evaluating the selected input limits. Although this approach is often used in trial scenarios, it has also been studied for its potential use in process visualisation and improvement (Wang et al., 2016).

Implementing a DoE has been the primary focus of Suykens et al. (2014), a method that uses objects to guide improvement by conducting an equitable evaluation of the selected input limits. There has been consistent evidence in the literature that this method can improve the performance of agitators for methane transformation and the performance of unit administrators for less-carbon hydrogen output systems, such as SE-SMR. Process model augmentation with DoE is valuable because it considers the equal evaluation of diverse data boundaries. To learn how certain significant limitations interact with the KPIs and what conditions lead to optimal performance, it is possible to use DoE in process display. Latin hypercube testing (LHS) is one computational methodology that has been the subject of ongoing research. LHS partitions the dataset into square networks, chooses outwardly irregular information, and guarantees fluctuation within the dataset by selecting a four-sided matrix containing statistics since line and section, respectively (Namoun et al., 2022).

Another famous drift indoors this multivariable technique is the progress of improvement calculations, such as genetic algorithm (GA). GA may provide a definitive approach to multivariable optimisation when combined with process demonstration. GA mimics the progression of nature in its optimisation calculations. The computation first generates an atypical population of arrangements. Each stage involves selecting a new group of people since the existing inhabitants are perceived as guardians and shape the future. An ideal account has been zeroed in on incorporating GA to improve an initial design for an ATR reformer across progressing populations (Deng et al., 2009). The first configuration was effective for ATR display, resulting in a 24.8% drop in operating temperature and a 27.2% improvement in CH_4 transformation. Improved impetus designs were optimised with a GA to get the highest possible H_2 production while maintaining the lowest possible wall temperature in the immediate vicinity. According to Zhu et al. (2020), the original plan's heat double-dealing was improved as the H_2 production considerably augmented through a 39.3% reduction in the extreme neighbouring barrier malaise.

Using hydrogen in energy components necessitates ultra-pure hydrogen see Figure 4, which in turn requires the development of new purging processes. Segmented cleaning cycles, such as those used in public service announcements and TSA screenings, are effective in the blue hydrogen domain. Disentanglements and assumptions are often made while employing standard interaction test systems, and progressing by altering critical working conditions. Regardless, the proving and improvement will be computationally time-consuming using typical techniques.

Because of its ability to significantly accelerate, ML plays a crucial role in developing digital twins for these cycles. By considering the complex aspects involved in the interaction, ML may accelerate substantially and aid the model in progressing through these cycles more accurately. AI calculations may identify designs and constantly improve process parameters to achieve perfect execution through exercise replicas with massive datasets of cycle figures. This, in turn, primes for better-quality effectiveness, condensed costs, and amplified H_2 transparency. Hence, AI is essential for developing numeracy doubles for blue hydrogen output and showing and improving the cycle.

It is common practice to confront several non-direct PDEs until they reach a cyclic consistent state while developing adsorption-based procedures related to blue hydrogen output (e.g., TSA and public service announcements). The computing speed of conventional showing and the subsequent OFAT method of handling improvement (responsiveness evaluation) is low. Using DoE with other advancement methods, such as GA, which accounts for improving chosen substances (MOO), provides a computationally rapid and accurate solution to improvement problems. A growing trend in the literature is combining ML with GA to enhance cycles, like H_2 purging.

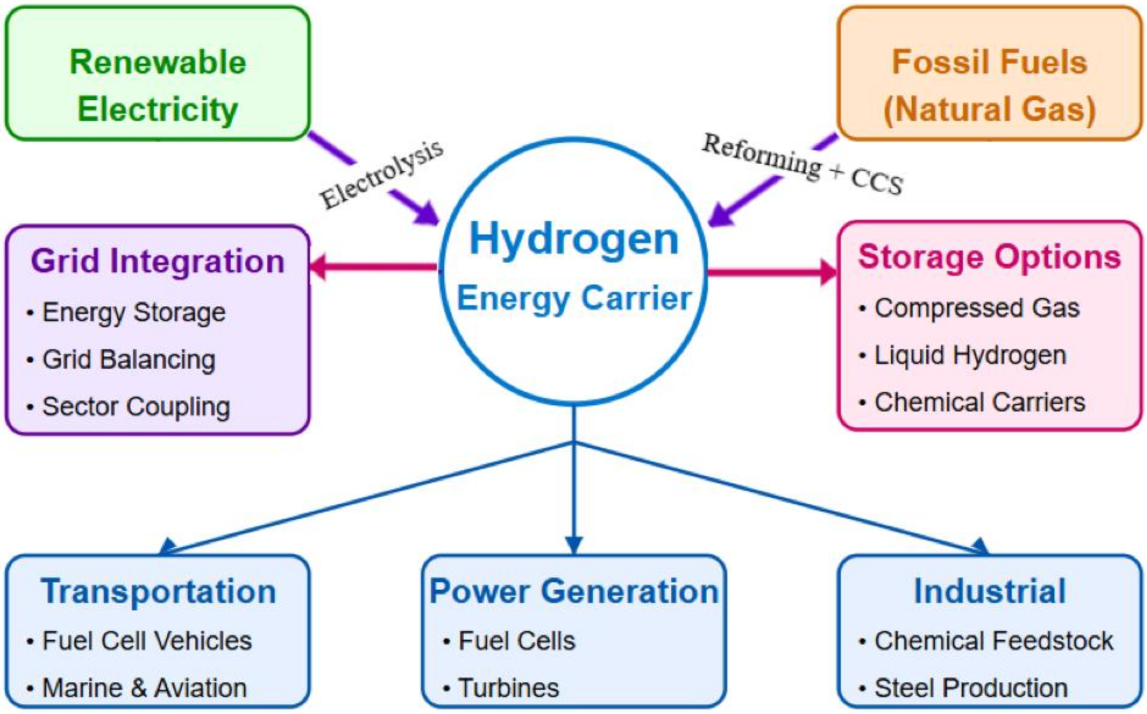

Figure 4. Hydrogen in Energy Components

4. A TECHNICAL OVERVIEW AND USE OF MACHINE LEARNING WITHIN H_2 MANUFACTURING

ML is reshaping blue hydrogen production by optimising processes, enhancing material development, and enabling predictive maintenance. ML algorithms analyse real-time data from various production stages, such as SMR and carbon capture, to identify patterns and optimise operating parameters for increased efficiency and reduced downtime. Additionally, ML accelerates catalyst and sorbent discovery through techniques like DFT and QSAR approaches, leading to higher yields and lower costs.

ML also enables predictive maintenance by analysing historical data to detect equipment degradation early, minimising unplanned downtime, and ensuring continuous operation. Furthermore, ML forecasts renewable energy availability, predicts CCS unit performance, and monitors plant operations for safety hazards and cyber threats, enhancing overall efficiency, safety, and security in blue hydrogen production. Through ML's capabilities, blue hydrogen production can become more sustainable, cost-effective, and resilient in the transition towards a cleaner energy future.

This segment initially starts through a concise clarification of the strategies and standards of ML and DL for the peruser to incorporate a viable understanding into the devices utilised in demonstrating, enhancing, and improving material inside blue hydrogen creation. The part then examines the new advancements in ML and how they have been consolidated in H_2 creation.

4.1 A Primer on Machine Learning

ML has transformed several sectors by providing sophisticated computer methods to evaluate intricate datasets and extract practical insights. In the field of hydrogen production, ML has great potential for optimising processes, increasing predictive skills, and raising overall efficiency (Vorontsov and Smirniotis, 2023; Şenol et al., 2024; Ramkumar et al., 2024). This section offers a comprehensive introduction to ML, emphasising its fundamental ideas, essential approaches, and particular applications in hydrogen production.

ML is a branch of AI that allows computers to acquire knowledge from data, recognise patterns, and make choices with no human involvement. The fundamental concept is to create algorithms that can derive general principles from a given number of instances, allowing the system to perform on novel, unfamiliar data properly. ML models may be classified into three main categories: supervised learning, unsupervised learning, and reinforcement learning.

Supervised learning: Supervised learning involves training a model using a dataset that has labelled examples, where each example is associated with an output label. The objective is to acquire knowledge of a transformation from given inputs to corresponding outputs, enabling the model to properly anticipate the result for novel inputs. Some commonly used techniques in ML include linear regression, logistic regression, decision trees, support vector machines (SVM), and neural networks.

Unsupervised Learning: Unsupervised learning involves analysing data without preexisting labels or categories. The goal is to deduce the hidden arrangement of the information without explicit output labels. This kind of learning is often used for tasks including grouping, reducing dimensionality, and detecting anomalies. Some important techniques include k-means clustering, hierarchical clustering, and principal component analysis (PCA).

Reinforcement Learning: Reinforcement learning is the process of teaching an agent to make a series of choices through its interaction with an environment. The agent is provided with feedback in the form of rewards or penalties, and the objective is to optimise the total accumulated reward over a period of time. This method is often used in robotics, gaming, and autonomous systems.

4.1.1 Neuronal Anatomy: Fundamental Organization

The fundamental principle of machine learning, namely neural networks, is centered on the artificial neuron, which draws inspiration from the organic neurons found in the human brain. An artificial neuron, often referred to as a perceptron, functions as the essential component of neural networks. Its design aims to replicate the manner in which organic neurons process and convey information. An artificial neuron consists of many essential elements: inputs, weights, bias, summation function, activation function, and output.

Inputs: The inputs to a neuron consist of the properties or qualities of the data that is being processed. A numerical value denotes each input, and together, these inputs constitute a vector. For example, in the process of generating hydrogen, the factors that are considered as inputs may include temperature, pressure, flow rate, and catalyst concentration.

Weights: Each input is assigned a weight, indicating the significance or intensity of that specific input. The weights are adjustable variables that are precisely adjusted throughout the training process. The purpose of the weights is to adjust the magnitude of the inputs, emphasizing more important characteristics and reducing the impact of less relevant ones.

Bias: The bias is an extra factor that is included in the calculation of the weighted sum of inputs. It permits the adjustment of the activation function's position, either to the left or right, which is essential for acquiring knowledge of intricate patterns. The bias enables the neuron to generate predictions even in the absence of any non-zero input data.

Activation Function: An activation function is a mathematical function that operates on the weighted sum of inputs from the summation function and generates the output of a neuron. This function incorporates non-linear elements into the model, allowing the neural network to acquire and represent intricate patterns. Popular activation functions include the sigmoid function, hyperbolic tangent (tanh), and rectified linear unit (ReLU). The selection of the activation function may have a substantial influence on the performance and training of the neural network. One example of a frequently utilised function is the ReLU, which is beneficial in addressing the vanishing gradient issue. This function enables quicker and more efficient training of Deep Neural Networks.

Output: The neuron's output is determined by applying the activation function to the weighted sum of inputs and bias. The output may take the form of either a continuous value, which is used in regression activities, or a probability score, which is employed in classification tasks. Within a neural network, the output of a single neuron may be used as the input for another neuron in later layers, enabling a hierarchical learning process.

4.1.2 Artificial Neural Networks

A neural network is a complex system of linked neurons arranged in layers, including an input layer, hidden layers, and an output layer. Every layer modifies the input data using weighted connections and activation functions to achieve a more abstract representation. Neural networks excel at jobs that require the analysis of intricate patterns, such as recognizing images and voices.

Input Layer: The input layer is responsible for receiving the unprocessed data, where each neuron represents a certain characteristic of the data.

Hidden Layer: The concealed layers carry out calculations and extract characteristics from the supplied data. They are responsible for acquiring knowledge about the complex patterns and connections present in the data. The number of concealed layers and the number of neurons in each layer are pivotal hyperparameters that impact the network's functioning.

Output Layer: The output layer is responsible for generating the ultimate prediction or categorization. In a regression issue, the output layer may be a solitary neuron that represents the anticipated value. In a classification task, several neurons may be used to indicate the likelihood of each class.

4.1.3 Training of Neural Networks

Training a neural network involves adjusting the weights and biases to minimize the error between the predicted output and the actual target values. This process is typically carried out using backpropagation, a supervised learning algorithm that calculates the gradient of the loss function with respect to each weight by the chain rule, iteratively adjusting the weights to minimize the loss.

Forward Pass: During the forward pass, the input data is propagated through the network layer by layer to generate the output. The weighted sum of inputs and the bias are passed through the activation function at each neuron.

Loss Calculation: The loss function measures the discrepancy between the predicted output and the actual target values. Common loss functions include mean squared error (MSE) for regression tasks and cross-entropy loss for classification tasks.

Backward Pass: The backward pass involves calculating the gradients of the loss function with respect to each weight using backpropagation. The gradients indicate the direction and magnitude of the weight adjustments needed to reduce the loss.

Weight Update: The weights are updated using an optimisation algorithm such as stochastic gradient descent (SGD), Adam, or RMSprop. These algorithms adjust the weights iteratively to minimise the loss.

Iteration: The forward pass, loss calculation, backward pass, and weight update steps are repeated for multiple iterations (epochs) until the network's performance stabilizes.

4.1.4 Convolutional Neural Networks (CNNs)

Convolutional neural networks (CNNs) are a specific kind of neural network that is specifically built to handle structured grid data, such as photographs. CNNs include convolutional layers, pooling layers, and fully connected layers, each with a specific role in the process of extracting features and learning.

Convolutional Layers: The layers in question use a sequence of filters (kernels) to process the input data, executing convolution operations that extract characteristics such as edges, textures, and patterns. The quantity and dimensions of these filters are crucial factors that govern the extent and precision of the feature maps produced.

Pooling Layers: After the convolutional layers, pooling layers are used to reduce the size of the feature maps. This procedure decreases the number of dimensions in the data while preserving the most essential information. Pooling aids in reducing computing complexity and mitigating overfitting.

Fully Connected Layers: Following the convolutional and pooling layers, the fully connected layers analyse the retrieved features in order to provide predictions. The layers function as the decision-making element of the network, combining the acquired characteristics to provide the ultimate forecast.

4.1.5 Application of Machine Learning in Hydrogen Generation

ML is used in hydrogen production for many purposes, including improving the efficiency of the process, predicting when maintenance is needed, and identifying any unusual occurrences. ML models may discover valuable insights that result in increased efficiency, decreased operating expenses, and better system dependability by using extensive datasets from hydrogen manufacturing processes (Obiora et al., 2024).

Process Optimisation: ML algorithms may enhance hydrogen production processes by determining the most favourable operating conditions. ML models may evaluate data from SMR or electrolysis processes to ascertain the optimal temperature, pressure, and catalyst conditions for maximum efficiency. As a consequence, this leads to increased production of hydrogen and reduced energy use.

Predictive Maintenance: ML models have the capability to anticipate equipment malfunctions and maintenance requirements by examining past data and detecting trends that suggest deterioration and damage. Predictive maintenance minimises operational interruptions and prolongs the durability of vital elements, guaranteeing uninterrupted and effective hydrogen generation.

Anomaly Detection: Anomaly detection systems have the capability to detect deviations from typical operating circumstances, enabling operators to promptly address and rectify small errors before they develop into significant difficulties. This improves the safety and dependability of hydrogen-generating systems.

Quality Control: ML may be used to check the quality of hydrogen production as well. ML models may use sensor data and output characteristics to analyse and guarantee that the hydrogen satisfies the necessary purity criteria, which are crucial for applications such as fuel cells.

4.1.6 Implementing Machine Learning Models

The implementation of ML models encompasses many stages: data acquisition, preprocessing, model selection, training, assessment, and deployment.

Data Collection: The first stage involves collecting pertinent data from hydrogen manufacturing procedures. This encompasses data from sensors, operational variables, and output evaluations.

Data Pre-processing: Raw data often includes noise, missing numbers, and discrepancies. Preprocessing procedures, such as data cleansing, normalisation, and feature extraction, are essential in order to adequately prepare the data for modelling.

Model Selection: Various ML algorithms may be used based on the unique application. CNNs are well-suited for data that is based on images, but RNNs are particularly well-suited for data that is based on time series. Supervised learning models are used for tasks that include labelled data, while unsupervised learning models are applied for the purpose of clustering and anomaly detection.

Training: The chosen model has been trained using pre-processed data. This process includes inputting the data into the model, fine-tuning the model parameters to minimise the loss function, and evaluating the model's performance using a distinct validation dataset.

Evaluation: The model that has undergone training is assessed on a separate dataset called the test dataset in order to determine its accuracy, precision, recall, and other performance parameters. Cross-validation methods may be used to guarantee that the model exhibits good generalisation to unfamiliar data.

Deployment: After being verified, the model is implemented in the hydrogen production system. The system consistently monitors and analyses data, offering real-time insights and suggestions for enhancing the process.

Although ML has notable advantages for hydrogen production, many obstacles remain. These factors include the need for extensive, top-notch datasets and the intricacy of incorporating ML models into current systems. Subsequent investigations should prioritise the development of more resilient and comprehensible models, enhancing approaches for gathering and preparing data, and investigating novel applications of ML in the domain of hydrogen generation (Maleki et al., 2024; Dahake et al., 2024).

To summarise, ML is a potent tool for enhancing the progress of hydrogen-generating technologies. Researchers and engineers may use ML algorithms to optimise operations, improve predictive maintenance, and guarantee high-quality hydrogen production. This primer has provided a concise overview of the core concepts of ML, essential approaches, and particular applications in hydrogen production. It establishes a strong basis for further investigation and discovery in this domain (Elumalai and Ravi, 2023; Lu et al., 2024).

According to Ullah et al. (2020), the expert advances within the environment using strategy and reward. Figure 5 illustrates how these consequences are interconnected within support learning. Referring to the specialist's feedback as a reward is standard practice. The expert often faces the dilemma of research vs. double-dealing, in which the specialist should discover fresh statuses while increasing the dividend. Fostering an ideal approach is vital to the success of support learning.

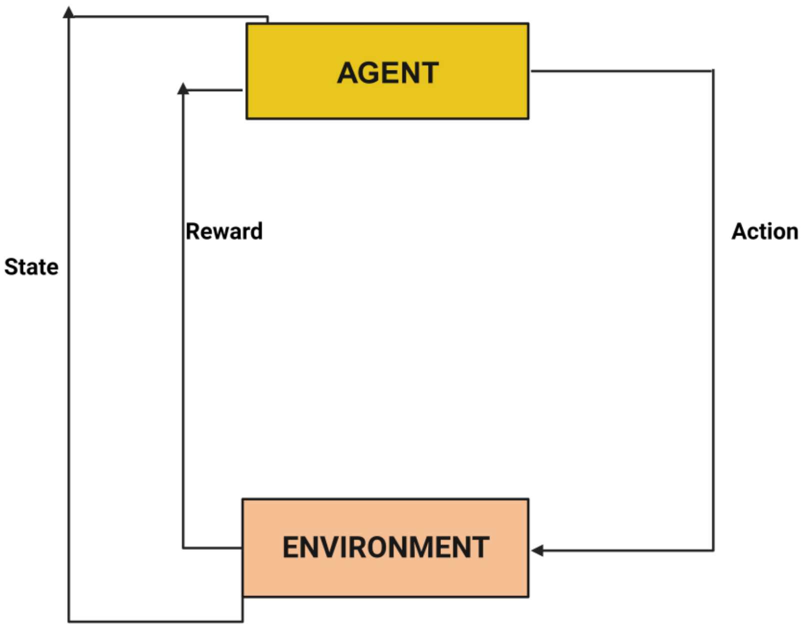

Figure 5. Reinforcement Learning Depicts the Agent's Interaction with Its Surroundings

AI gives experts tools to show very indirect rules. Using key variables in STEM-related domains requires considering the model's interpretability and other ethical considerations (Velis et al., 2023). However, the presentation of these cycles uses other ML processes, which effectively modify interpreted and analytical performance (Kannangara et al., 2018). In low-carbon hydrogen production, reproduction nervous links have been extensively used in the literature due to their design versatility. The following section will focus only on brain organisations and Deep Learning (DL) approaches, outlining their improvement over the last decade due to the extensive usage of these tactics in writing.

4.2 Artificial Neural Networks

ANNs are a prominent nonlinear modelling structure that imitates the functioning of the human brain. These systems are specifically designed to identify patterns, categorise information, and provide forecasts via the process of learning from given instances. ANNs are composed of linked nodes, also known as neurons, that are arranged in several levels: input layers, hidden layers, and output layers. Every individual node inside a layer is linked to nodes in the next layer by connections that have assigned weights. These weights are modified as part of the training process in order to reduce mistakes in predictions.

Regarding the production of hydrogen, ANNs provide notable benefits since they can effectively represent intricate and nonlinear connections among different factors in the process. These networks may be taught to forecast hydrogen output, optimise operational parameters, and detect abnormalities in real-time, therefore improving the efficiency and dependability of hydrogen production systems.

Training of Neural Networks: Training an artificial neural network entails optimising the weights of the connections between neurons to reduce the discrepancy between the expected output and the desired goal values. The method is often performed using backpropagation, a supervised learning algorithm that repeatedly adjusts the weights to minimise the loss by calculating the gradient of the loss function with respect to each weight using the chain rule.

During the training process, the input data is sent to the network, and the predicted output is evaluated against the actual target values. The discrepancy (mistake) is sent retroactively across the network, and the weights are adjusted correspondingly. This procedure is iterated over numerous epochs until the network's performance reaches a stable state, indicating that it has successfully acquired the ability to reliably translate the input data to the intended output.

Figure 6, depicting a traditional neural network, is crucial for understanding the basic architecture and operation of Convolutional Neural Networks (CNNs) in hydrogen production models. Figure 6 provides a graphic representation of how input data, such as sensor readings and process parameters, is converted via many levels to generate an output, such as hydrogen yield and efficiency metrics, in the context of hydrogen production. The convolutional layers seen in Figure 6 are significant because they demonstrate how CNNs may acquire hierarchical representations of data. Regarding the production of hydrogen, these representations might include the identification of the most favourable operating circumstances, the detection of abnormalities, or the prediction of system performance in different situations.

The convolutional layers seen in Figure 6 are specifically intended to capture complex patterns and interconnections within the input data. Through the application of filters to the data, these layers have the ability to detect and analyse crucial characteristics that have an impact on hydrogen generation processes. The hierarchical feature extraction capabilities of CNNs can successfully mimic temperature and pressure fluctuations, which are key factors in hydrogen production. This facilitates a more precise and all-encompassing comprehension of how various factors interrelate and impact the overall functioning of the system.

The architecture of CNNs is shaped by several parameters, most notably the selection of the number and dimensions of the convolutional layers.

Nature of Input Data: The input data for hydrogen production consists of time-series sensor readings, temperature measurements, pressure data, and other process parameters. The convolution layers are required to capture both the temporal and spatial relationships present in this data. When dealing with jobs that involve extracting specific features, such as detecting anomalies or forecasting hydrogen yield in complicated situations, deeper networks with an increased number of convolution layers may be required. In contrast, less complex activities may need a network with fewer layers.

Complexity of the Task: The network design is determined by the intricacy of the hydrogen-generating process. For instance, when attempting to represent non-linear connections between process variables, it may be necessary to use numerous layers in order to correctly capture the complex interdependencies.

Computational Resources: The computational burden is affected by the size of the convolution layers, which includes the number of filters and their diameters. Increased filter size and quantity enhance feature extraction capabilities, but more processing power and memory are needed. Ensuring a harmonious equilibrium of these aspects is important in the development of models that are both efficient and successful.

Empirical Tuning: Frequently, the structure of CNNs is optimised by practical trial and error. Cross-validation and hyperparameter optimisation methods are used to ascertain the most suitable number and dimensions of convolution layers. This empirical methodology guarantees that the model is customised to the distinct attributes of the data and the demands of the job.

When building CNNs for simulating hydrogen production, it is crucial to take into account the precise requirements of the application. For example, to accurately capture the quick changes in sensor readings during hydrogen generation, it may be necessary to use a larger number of convolution layers with smaller filter sizes. This will allow for more detailed extraction of features. However, when it comes to modelling long-term trends in production efficiency, it may be necessary to use bigger filters and pooling layers in order to capture more extensive patterns.

The use of CNNs in the modelling of hydrogen production is very pertinent because of their capacity to process intricate and extensive information effectively. Hydrogen-generating methods consist of many steps, each characterised by specific characteristics and operating circumstances. CNNs can autonomously extract pertinent characteristics from unprocessed sensor data, recognising patterns linked to effective hydrogen generation or spotting departures from typical operational states.

CNNs are very effective at representing the complex and non-linear connections between variables in hydrogen production processes. These models provide valuable insights into the correlation between changes in process parameters and their influence on hydrogen production and efficiency. By using the hierarchical feature extraction capabilities of CNNs, predictive models may get enhanced accuracy in predicting hydrogen production metrics. This is essential for optimising processes and minimising operational expenses.

Moreover, the capability of CNNs to efficiently handle data in real-time renders them very suitable for the surveillance of hydrogen-producing systems. They can promptly offer feedback on the functioning of the system and notify operators of any problems before they become more serious, thus improving the overall reliability and efficiency of the system. The capacity to interpret data in real-time is very useful in the field of hydrogen generation, as it allows for quick modifications to operating parameters that may have a substantial influence on overall efficiency and output.

To summarise, the use of CNNs in hydrogen production modelling is crucial for enhancing prediction precision, streamlining procedures, and facilitating live monitoring. CNNs may be efficiently used to improve hydrogen production systems by strategically choosing the number and size of convolution layers, taking into account factors such as the characteristics of the input data, job difficulty, processing resources, and empirical tuning. Figure 6 is crucial in elucidating these notions, offering a clear and exhaustive comprehension of how CNNs may convert unprocessed data into practical insights for hydrogen creation.

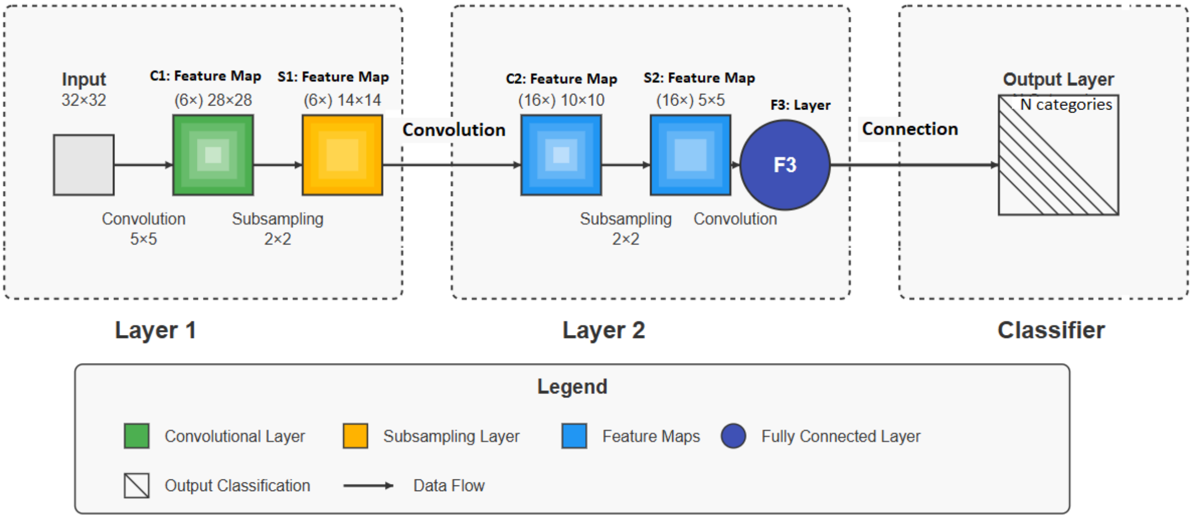

Figure 6. Convolutional Neural Networks

In the context of blue hydrogen production, ML has gained prominence for its ability to optimise processes, enhance material development, and enable predictive maintenance. ML algorithms analyse data from various stages of hydrogen production, such as steam SMR and carbon capture, to improve efficiency and reduce downtime. ML also accelerates the discovery of catalysts and sorbents, leading to cost savings and higher yields. However, recent trends indicate a shift towards developing brain networks capable of modelling complex cycle designs (Wang et al., 2024). Brain networks, which have been utilised since the 1940s, were previously overlooked due to a focus on other ML methods. However, with advancements in CNN technology, there has been a resurgence of interest in brain-inspired approaches. This includes leveraging DL and large datasets to enhance ANN performance (Arsad et al., 2023).

The key components of a neural network include the input, hidden, and output layers. Information is processed through these layers, with the output layer generating results based on the input data and context. Brain networks aid in this process by calculating and focusing on crucial features within the data, contributing to improved model performance (see Figure 7).

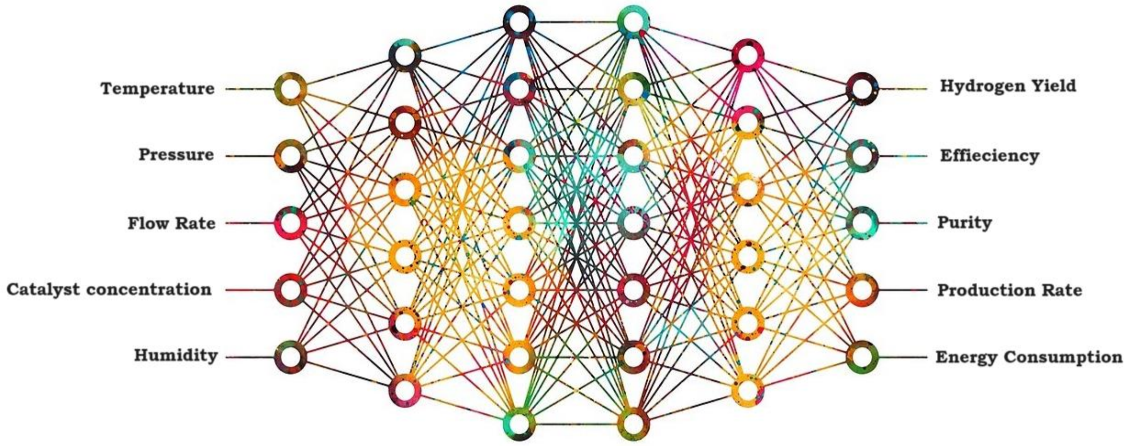

Figure 7. Basic Structure of a Neuron

4.2.1 Training of Neural Networks

Respectively, the neuron obtains a replica of the data sources and irregular loads (refined during development). Each neuron's loads and contributions since the earlier film stay directly combined and multiplied by a static inclination value. The appropriate initiating capability selects the neuron's final value (Fei et al., 2021). Equation (1) illustrates this:

$$z = \sum X_n W_n + b \quad (1)$$

where z = neuron, X_n = input data, W_n = weight for each data point.

Within the domain of blue hydrogen production, various ML techniques are employed, depending on the characteristics of the data values. Essential among these is the activation function, which determines when a single neuron remains inactive or becomes active (Zeng and Jia, 2024). This function introduces non-linearity into the framework, which is crucial for tasks such as DL. Subsequently, the loss function is calculated to assess the accuracy of the model (Gul et al., 2024). Non-linear activation functions, like ReLU, facilitate DL by enabling the model to handle complex relationships within the data.

ML aims to minimise the likelihood of errors, ensuring that the model's output aligns with the patterns observed in the training data. Typically, this involves utilising gradient descent methods to minimise the loss function. Gradient descent calculates the slope from a random starting point and adjusts the learning rate dynamically to optimise the descent process.

Data is typically divided into three parts when constructing a neural network model: training, validation, and testing. The majority of the data is used for training, where the model learns from examples and fine-tunes hyperparameters. The validation set is then used to assess the model's performance and prevent overfitting, ensuring that the model generalises well to unseen data. Finally, the testing set contains data used to evaluate the effectiveness of the trained model.

In determining the proportions of training, validation, and testing data, various factors must be considered. There is no "one-size-fits-all" rule for dividing the dataset, and careful consideration is needed to ensure the model's robustness and generalisation capabilities.

4.3 Advancements in Machine Learning

ML is undergoing a revolution. Fuelled by expanding datasets, robust processing power, and innovative algorithms, advancements are occurring rapidly across various domains. From mastering intricate games like chess to unravelling complex protein structures, machines are demonstrating increasing intelligence and problem-solving abilities. These advancements are not confined to research laboratories; they are already impacting daily life, from personalised recommendations to autonomous vehicles, with progress showing no signs of slowing. As ML continues to progress, the potential for breakthroughs in healthcare, materials science, climate change mitigation, and beyond appears limitless, positioning it as one of the most exciting and transformative technologies of our era (Magazzino and Zoundi, 2025). In the last 20 years, ML has grown as a subject of study and has been used in various industries. This section discusses the progressions inside the cycle design and STEM-based study settings.

4.3.1 Recent Progress in Neural Networks

In recent decades, a wide range of brain networks have been developed that are tailored to specific tasks. The most recent developments in neural networks are summarised in Table 4, providing brief descriptions of each type.

Table 4. Typical Neural Networks

Neural Network	Description
Neural Networks that use feed-forward	Data flows unidirectionally from input to output in the most basic neural network architecture, which does not include DL methods such as backpropagation or automated feature extraction.
Reinforcement learning system (RNS)	According to Mann et al. (2023) and Kanrar and Sarkar (2024), the output of one layer may be input to subsequent levels. Simple RNNs suffer from problems like vanishing gradients, but their design makes them ideal for time-sequence data and sequential learning.
Long-short term memory (LSTM)	While LSTMs are comparable to RNNs in that they can store data, they differ in that LSTMs use a "forget gate" to prevent problems like vanishing gradient, which is prevalent in RNNs. According to Wang et al. (2016), LSTM has been found to be extensively used in video data processing.
Deep Learning system	A convolution operation is performed on the input vectors by neurons organised in 3D layers.
Interconnected Neural Networks	Separate networks do not communicate with one another but rather operate autonomously to produce a result.

4.3.2 Innovations in Deep Learning

In the realm of ML, DL has emerged as increasingly crucial, particularly in the past decade. Complex neural networks with multiple layers are utilised to analyse vast datasets (Farfán et al., 2024). DL is particularly effective for handling chaotic and unstructured datasets, as it automates feature extraction and model construction (Ye et al., 2024). These networks consist of progressive neurons that employ forward-thinking behaviours, enabling them to glean valuable insights from scarce data, such as in robotic feature extraction (Peksen and Spliethoff, 2023).

A recent innovation in ML is the introduction of physics-informed neural networks (PINNs), which leverage domain knowledge to inform network architecture and decision-making (Cheng et al., 2024). PINNs utilise prior knowledge to identify optimal configurations, taking into account biases inherent in the learning process. These networks prioritise robustness and the ability to handle complex scenarios, making them well-suited for tasks such as blue hydrogen production optimisation. By integrating PINNs into advanced computational models, such as digital twins, the fusion of data with accurate physics-based models can significantly enhance compound design processes.

4.3.3 Ensemble Learning

A fresh growth in ML exploration is group recognition, which entails combining the predictions given by several models and condensing many ML computations. Suvarna et al. (2022) showed that it is more accurate than examinations using a single ML computation. One projecting sample of an outfit erudition technique that syndicates many conclusions to create an expectation is RF. Multiple methods exist for various ML calculations, such as stacking, bagging, and boosting.

4.4 What Is the Purpose of Using Machine Learning in Hydrogen Production, and How Is It Implemented?

The utilisation of ML in hydrogen production aims to optimise processes, enhance efficiency, and reduce costs. ML algorithms analyse extensive datasets gathered from various stages of hydrogen production, including SMR and CCS, to identify patterns and optimise operational parameters. Through continuous learning from operational data, ML algorithms can adapt and improve over time, leading to enhanced performance and minimised downtime. Additionally, ML facilitates predictive maintenance by analysing historical data to detect equipment degradation early, thereby minimising unplanned downtime and ensuring continuous operation. Moreover, ML enables the discovery of new catalysts and sorbents through techniques like DFT and QSAR approaches, resulting in higher yields and lower costs. The integration of ML algorithms into existing infrastructure and control systems enables real-time monitoring and optimisation of production processes. ML also enhances the exhibition of chemical cycles and specifically aids in H_2 production, improving data collection and analysis through methods like PCA. Furthermore, ML models, often developed using ANNs, are refined using techniques like GA to optimise model performance and identify optimal operating boundaries. Understanding how ML models adapt, particularly in complex cycles like H_2 production, is crucial for ensuring accurate and robust models. Additionally, mathematical methods are employed to enhance the efficiency of arrangements within the process.

5. BLUE HYDROGEN GENERATION USING MACHINE LEARNING: AN IMPORTANT OUTLOOK

This slice examines the similarities in dark and blue hydrogen ML model cycles. From initial material screening and improvement to full plant expansion, we have researched and analysed ML use in various hydrogen output procedures. In this way, we have shown how ML is currently used and recognised zones where it might be long drawn out in producing blue hydrogen. A research overview of ML within hydrogen production is presented in Table 5.

Table 5. A Research Overview of Machine Learning Within Hydrogen Production

Reference	Overview	Results and Model Overview
Namoun et al. (2022)	The LHS technique acquired data for model training, testing, and validation using intricate mathematical software. Using a GA algorithm on both ANNs, we improved the PSA column's operational performance by producing optimum solutions.	One ANN model with five inputs (adsorption pressure, time, feed flow rate, activated carbon layer length, and purge-to-feed ratio) and two outputs (purity, recovery), R^2 (0.999970), MSE (1.165×10^{-6}). Five inputs, three outputs (purity, recovery, productivity), R^2 (0.999950), MSE (1.1164×10^{-4}) in ANN Two. Utilising ANNs as surrogate models for the optimisation framework is accurate and considerably reduces optimisation time.
How et al. (2020)	Their method optimises an eight-step PSA cycle for pre-combustion CO_2 collection. The model was trained, tested, and validated using MATLAB first-principle process modelling data. Four ways existed. Tradopt adapted a GA to the first-principle PSA model built in MATLAB, whereas SOpt applied it to ANN.	TradOpt processing time was lowered by 90% using SOpt. The model is precise. DRopt significantly cuts time (~50%) compared to other methods. DR-SOpt speeds up high-purity H_2 operating parameter generation.
Krogh (2008)	Dynamic models were combined to predict the process's performance, producing high-purity H_2 and a CO_2 capture rate of 90%. An ANN was developed for each unit to determine the optimum operating conditions for this process, achieving a marginal error of <2% and a low computational cost of <12s.	The process-driven model optimised H_2 production cost from 2.045 $/kg to 99.99% purity and 91% CO_2 capture rate at 1760 m^2 membrane area, 387 s adsorption time, and 0.106 purge-to-feed ratios.

5.1 Applying Machine Learning to the Creation of Materials for Hydrogen Production

Applying ML to the creation of materials for hydrogen production offers various benefits, such as subatomic displays of catalysts and resources for CO_2 imprisonment using DFT estimates and atomic elements, as shown by Kabir et al. (2023). Another example is the differentiation of resources for specific capabilities based on their construction. This approach has gained attention due to the high cost of platinum catalysts, with works by Kumari et al. (2024) focusing on using ML within DFT estimates to discover new catalysts. Traditional atomic display methods are typically used for materials screening, but the use of PCA in conjunction with ML-based QSAR evaluation can enhance material combinations. Recognising critical underlying boundaries impacting attributes and feeding them into a neural network can help determine materials with the best speed and accuracy. Moreover, future research should focus on improving interpretability within ML-assisted QSAR, ensuring a robust system capable of efficiently assessing materials when properly configured.

5.2 Hydrogen Manufacturing Process Modelling Improved Using Machine Learning

ML has been applied to blue hydrogen output to enhance overall cycles, streamline individual interaction units, and increase the sensitivity of different cycle units. The goal is to achieve outcomes such as H_2 virtue and CH_4 change. In what follows, an example of a pattern that uses ML within the process is provided, and it uses ANN and GA to streamline individual cycle units and complete cycles. Additionally, the emergence of crossover demonstration and the reasons behind it are examined, which takes into account improved execution while maintaining accuracy and interpretability. Next, we look at how ML has been used in the last five years and how it will continue to be used in the H_2 production process.

5.2.1 Analysis of Traditional Process Modelling Methods Compared to Machine Learning-Based Methods

The use of ML to increase blue hydrogen output procedures, whether through the demonstration of individual interaction units or the augmentation of complete cycles, has been the focus of most of the work. For instance, PSA segments are particularly laborious to recreate because process units like these are extreme cycles; as a result, improving itemised and dynamic cycle models is a long process. Table 6 presents the time and accuracy required to simulate blue hydrogen manufacturing units and processes using ML.

Table 6. Time and Accuracy Are Required to Simulate Blue Hydrogen Manufacturing Units and Processes Using Machine Learning

Reference	**Unit**	**ML algorithm**	**Model Accuracy in ML**	**Approach to optimisation**	**Time for optimal modelling**
Abdin (2024)	PSA	FNN with BP	MSE: 1.16419E-04 R^2:0. 995%	GA	32.07 s
Yang and Yang (2014)	PSA	FNN with BP	MSE: 1.36581E-06 R^2: 0.997%	GA	176.13 s
Abdulkadir et al. (2012)	PSA	FNN with BP	RMSE: ~0.20 R^2: 0.98	GA	~400 core hours
Davies et al. (2023)	PSA	Partial Least Squares (PLS)	RMSE: 1%	GA	~2000 core hours
Karri et al. (2008)	P.S.A.	FNN with BP and PLS	RMSE: ~0.15	GA	~600 core hours
Abdallah et al. (2020)	Cryogenic Process	FNN with BP	R^2: 0.9976	GA	<12 s
Gadanidis (2017)	Membrane	FNN with BP	R^2: 0.9856	GA	<12 s
Khalaf et al. (2024)	SE-SMR process	Hybrid model	SD<2%	GA	<25 s
Adeleke et al. (2021)	Reformer	FNN with BP	R^2: 0.9891	GA	2 s

Table 7 displays the typical interaction showing the recreation season of cycle components and entire cycles of hydrogen output; in each instance, the reenactment runs much slower than its ML counterparts. Even though it provides interpretability, this white-box approach to demonstration is fundamentally slower. This is because it frequently encounters various non-direct PDEs until it reaches a cyclic consistent state, which is necessary for displaying the powerful presentation of a public service announcement unit. It is possible to replicate the cycles of creating public service announcements and H_2 more quickly with the help of ML.

Table 7. Time Required to Simulate Blue Hydrogen Manufacturing Units and Processes Using Traditional Methods

Reference	Unit	Model for process type	Type of optimisation
Wang et al. (2024)	PSA	Innovative	GA
Farfán et al. 82024)	Reformer	Innovative	GA
Zeng and Jia (2024)	SE-SMR Process	Innovative	GA

Nonlinear autoregressive regressions with external data sources (NARX) is an indicator structure used in nonlinear frameworks, such as brain organisations. According to Adedeji and Wang (2019), NARX is prone to errors associated with input estimations since it depends on previous estimates of data and results. The cumulative effect of the error makes NARX less useful for long-distance reenactments.

5.2.2 Soft-Sensor Development

Because they provide insight into difficult-to-decide data that regular sensors cannot, delicate sensors are a resource for endless cycles due to their ability to provide continual data, subject to managing situations. Analysing RF and ANNs for sensitive sensors used in the SE-SMR reformer and calciner, Morrow and Rondinelli (2002) showed that these sensors helped produce blue hydrogen. By shedding light on the interaction, it considers enhanced process control, which is already a challenging decision-maker. More effort is needed to ensure that sensors are adequately tested and validated before being implemented into certified applications and that errors are minimised. Applying Monte-Carlo techniques inside the preparation cycle is one novel approach to this problem.

The interpretability of these models is a critical concern in their applications in synthetic design. Such models can access an enormous database and properly present connections based on accuracy since they are trained on noteworthy writing data or pilot plants (Lombardo et al., 2022). Completed information from a first-guideline perspective may help us understand the functional components that propel the cycle to produce an extremely pure H_2 surge while maintaining a high CO_2 collection rate. The process results in traditional software-based demonstrations like gPROMS or Aspen, depending on first-principles conditions (changes in mass and intensity), thermodynamic and dynamic data, and a white-box rendering method.

5.2.3 Hybrid Modelling

The ML-based model's enhanced interpretability is considered during the cross-breed presentation. This middle ground has been discussed in writing as an essential step forward in reenactment (Oguz-Ekim, 2021). Integrating partial differential equations (PDEs) into a neural network to display hydrogen cycles could provide significant benefits, such as vulnerability evaluation, speed, and power of models, as well as more interpretability to rigorous ML-based models; this is a new development in ML within the natural sciences.

5.3 Digital Replication and Artificial Intelligence for Improving Entire Facilities

Enhancing entire facilities through digital replication and AI is crucial for maximising the benefits of certain blue hydrogen advancements like SE-SMR, despite their relatively low Technology Readiness Level (TRL). While dark hydrogen has already reached the scale necessary for industrial deployment, significant upgrades are required for SE-SMR. In Spain, a notable example involves the utilisation of ML to optimise an entire SMR facility. Researchers, as described by Ramesh et al. (2023), implemented a measured brain organisation to upgrade the facility, aiming to increase hydrogen purity and overall plant profitability. However, due to the early stages of these advancements, there is a necessity for a substantial dataset suitable for training neural network models, and currently, limited work has been done utilising plant data.

5.4 Blue Hydrogen Generation Using Machine Learning: Where Do We Go From Here?

The use of AI in H_2 production has had a profound effect. Table 8 below lists the pros and cons of utilising ML within H_2 for all display sizes. The chart also suggests areas needing additional research to fully include ML in hydrogen generation.

Table 8. Pros and Cons of Integrating ML Into Hydrogen Production

Scale of modelling	Positive aspects	Negative aspects	Future studies enhancements
Physical Dimensions	Accelerated progress in materials science	It is necessary to enhance the comprehension of the ANN-based QSAR framework	Assessing substances and optimising their manufacturing effectiveness in tandem
Dimensions of the Procedure	Modelling is completed much more quickly than with more traditional methods. Improvements in passive sensors have made it possible to optimise processes in real-time. GA provides an outstanding and reliable structure for optimising PSA units coupled with ANNs.	Using just ML for understanding decreases the procedure's comprehension. Different neural network architectures might result in differing model results despite the fact that they provide more flexibility. The purpose of your model should guide your careful evaluation of neural network design.	Creation of soft-sensor models using random modelling and instruction. Improving models' predictive power with combined learning Hybrid modelling further develops a hybrid approach to ensure high speed while maintaining interpretability. Applying RL to enhance safety in H_2 manufacturing operations and creating innovative methods for producing low-carbon hydrogen.

ML can provide faster display without sacrificing accuracy. Various display scales have been used, ranging from the subatomic to the cycle and even the complete plant scale. Much research has focused on public service announcements and TSAs to improve sensitive sensors for this interaction and shorten these cycles using ML, particularly artificial neural networks. According to Bijos et al. (2022, it is essential to carefully consider the purpose of using the brain network and its architecture when making decisions on the brain's structure. Although this was implemented for the Fischer-Tropsch process, comparable criteria are also applicable for the H_2 purging cycles.

6. CONCLUSIONS AND POLICY IMPLICATIONS

In conclusion, blue hydrogen emerges as a crucial component in achieving net-zero emissions by 2050. The paper identifies three key areas where advancements in technology are driving progress in blue hydrogen production: the development of new materials for CO_2 capture, the use of sensitive sensors to enhance process execution, and the implementation of dynamic display systems to improve efficiency in hydrogen purification. ML plays a pivotal role in accelerating these advancements by enabling faster discovery of materials and simplification of procedures. As the urgency of addressing climate change grows, the need for rapid innovation becomes increasingly evident. Future research should focus on leveraging ML to expedite the synthesis of blue hydrogen generation materials and optimise production cycles without sacrificing comprehension. By integrating ML seamlessly into existing infrastructure, the potential for achieving a low-carbon future through blue hydrogen production is significantly enhanced. The paper underscores the transformative impact of ML in revolutionising hydrogen production and underscores the importance of continued research and development to fully harness its capabilities in advancing sustainable energy solutions (Magazzino, 2023).

This study presents a comprehensive integration of AI, particularly ML, into blue hydrogen production systems. Unlike previous works that focus either on material discovery or process optimisation in isolation, this paper uniquely combines both domains by employing AI to link catalyst/sorbent development with system-level process modelling, thereby offering a holistic blueprint for next-generation hydrogen production.

Quantitatively, AI-driven models demonstrate significant reductions in simulation and optimisation time, up to 90% compared to traditional methods, while maintaining high predictive accuracy for H_2 purity and CO_2 capture efficiency. Qualitatively, the study introduces hybrid modelling strategies that merge AI with first-principles methods, improving interpretability without compromising speed.

Practically, the integration of digital twins and soft sensors powered by AI presents immediate opportunities for real-time optimisation, predictive maintenance, and cost-effective scale-up in industrial hydrogen facilities. These insights are especially relevant for sectors targeting low-carbon transitions, including power generation, transportation, and chemical manufacturing.

Broader impacts of this research include its applicability to renewable energy systems, where hydrogen acts as a critical energy carrier and storage medium. The framework proposed here can also be adapted to green hydrogen systems and extended to other decarbonisation pathways such as ammonia production or synthetic fuels.

Future research should explore adaptive AI models trained on real-time industrial data, the development of interpretable AI systems, and cross-sector collaboration to ensure policy, technology, and workforce development evolve in tandem.

The following relevant policy implications can be highlighted:

- Establish open data standards and sharing platforms: Governments and research institutions should promote open-access data repositories for hydrogen production and CCS processes to support AI model development and benchmarking.
- Support pilot projects integrating AI with hydrogen plants: Targeted funding should be allocated for demonstration projects that incorporate AI-driven monitoring, predictive maintenance, and process optimisation in existing blue hydrogen facilities.
- Incentivise the development of digital twins: Regulatory bodies should encourage the development of digital twin infrastructure for hydrogen systems by providing R&D tax incentives or grants, particularly for early-stage AI-integrated designs.
- Integrate AI into national hydrogen strategies: National hydrogen roadmaps should explicitly identify AI and machine learning as enabling technologies, with clear funding streams, regulatory frameworks, and technical standards for deployment.
- Encourage cross-sector collaboration: Foster partnerships between AI researchers, hydrogen technology developers, and policymakers to ensure models are not only technically robust but also aligned with industrial and regulatory needs.
- Prioritise skills development in AI and energy systems: Develop specialised training programs that bridge the gap between data science and hydrogen technology to create a skilled workforce capable of implementing and managing AI-driven solutions.

Despite the considerable promise AI brings to hydrogen production, several challenges must be acknowledged. First, the quality and availability of high-resolution operational data remain limited, particularly for full-scale industrial hydrogen systems. This can hinder the training and generalizability of ML models. Second, scalability remains a concern, as models trained on small-scale or lab-based systems may not always translate effectively to larger industrial operations. Third, integrating AI solutions into existing infrastructure and control systems can pose technical and organisational challenges, especially in facilities that rely on legacy technologies. Addressing these hurdles requires coordinated efforts in data acquisition, model robustness, cross-disciplinary collaboration, and regulatory guidance to fully realise AI's transformative potential in the hydrogen sector.

DECLARATIONS

Competing interests The authors declare no competing interests.

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