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Recent trends in sustainable modelling for hydrogen production and utilization

April Lia Hananto¹, Abdullahi Tanko Mohammed², Permana Andi Paristiawan³, Ihwan Ghazali^{4*}, Muhammad Idris⁵, Syah Alam⁶, Mega Tri Kurnia⁷

¹Faculty of Engineering and Computer Science Universitas Buana Perjuangan Karawang Teluk Jambe, Karawang 41361, Indonesia

²Department of Mechanical Engineering, Waziri Umaru Federal Polytechnic Birnin Kebbi, Nigeria

³Research Center for Metallurgy, National Research and Innovation Agency, South Tangerang, Banten 15314, Indonesia

⁴Fakulti Teknologi Kejuruteraan Mekanikal dan Pembuatan, Universiti Teknikal Malaysia, Melaka, Hang Tuah Jaya Durian Tunggal 76100, Melaka, Malaysia

⁵PT PLN (Persero), Engineering and Technology Division, Jakarta, Indonesia

⁶Department of Electrical Engineering, Universitas Trisakti, Jl Kyai Tapa No 1, West Jakarta, Indonesia

⁷Department of Computer System, Faculty of Computer Sciences, Universitas Bung Karno, Jl. Kimia No 20. Menteng, Jakarta 10320, Indonesia

*Corresponding author: ihwan@utem.edu.my

Abstract

Hydrogen is a promising candidate for the future of energy and global economic security owing to its cost-efficient clean and environmentally friendly nature. The utilisation of hydrogen is, however, not without obstacles. Technology maturity and the unattractive market are some of the challenges. Before hydrogen can be used on a large-scale basis, critical technical challenges need to be addressed, such as the economical production and transportation and storage issues. In terms of energy prices, hydrogen is an inexpensive fuel. Ideally, a vehicle run on hydrogen reduces the cost per kilometre with better mileage than that of fuelled with fossil fuel. Electric vehicles run on hydrogen fuel cells, for instance, offer several performance improvements over conventional internal combustion engines. This includes better fuel efficiency and relatively less noise operation, yet one of the important technical challenges is onboard hydrogen storage. In this review article, recent trends in modeling for hydrogen production and utilization are addressed in detail.

Keywords: Hydrogen production, renewable energy; hydrogen storage, modelling, future energy.

1 Introduction

Today, the development of alternative energy, such as biofuels and hydrogen, is attracting a great deal of attention worldwide [1-3]. Hydrogen energy is considered the most promising clean energy for the 21st century, attracting considerable interest from researchers, government agencies, and policymakers throughout the world [4, 5]. Unfortunately, just above 95% of hydrogen was

produced from non-renewable sources in 2018, and the most widely used processes were natural gas reforming (nearly 50%), oil reforming (30%) and coal gasification (18%) [6].

Attempts to protect the environment have led to the development of cleaner and renewable energy for a global sustainable economy. For this purpose, hydrogen as 'energy carrier' has long been considered a promising choice for energy storage and transportation [7, 8]. The combustion of hydrogen does not release CO₂ and pollutants into the environment. H₂ can be converted into electricity in fuel cells. Hydrogen is also the source of numerous industrial processes, such as the production of ammonia and methanol. Today, the global consumption of hydrogen is approximately 70 Mton/year [7].

Hydrogen is considered to be a promising energy carrier for decarbonization and energy security. Today, the most fundamental and profitable industrial process for the purest form of hydrogen production is obtained by electrolysis of water, where water is decomposed into oxygen and hydrogen gas by circulating electricity [9]. The minimum voltage required for the electrolysis of water at 300 K is 1.23V, with a range of 1.5 to 1.9V for real operation. Current water electrolysis technologies have efficiencies in the range of 70% and 90% [10]. Catalysts are employed to increase the reaction rates. Research and development are currently being investigated to increase electrolysis efficiency and to develop more efficient and inexpensive catalysts. Despite many options available, Jia et al. [11] used platinum black (cathode) and iridium black (anode) with an efficiency of over 30% solar to hydrogen.

2 Discussion

2.1 Hydrogen Energy: Global Interest

A hydrogen economy is beneficial for any country. In America, Rodriguez et al. [12] carried out an evaluation for hydrogen production using wind energy in Cordoba, Argentina. Posso et al. [13, 14] examined and estimated the potential for hydrogen production using renewable resources in Ecuador and Venezuela. Levene et al. [15] examined the potential of hydrogen production from water electrolysis of water employing energy produced from wind and solar in the USA. In Asia, Ni et al. [16] investigated the potential for hydrogen production from biomass, solar, and wind in Hongkong. In Europe, Siyal et al. [12] evaluated hydrogen production using wind energy in Sweden. Dagdougui et al. [17] introduced a method to determine and select the appropriate locations for hydrogen production from different sources, such as solar and wind through water electrolysis in northern Italy. In Africa, several studies have been conducted to evaluate the potential for the production of hydrogen in Algeria [18-20]. Honnery et al. [21] evaluated the potential global hydrogen production potential.

2.2 Hydrogen-powered vehicle

Hydrogen-powered vehicles (HPV) are also another promising technology [22]. Various investigations on HPV have been conducted. Chen et al. [23] proposed a novel two-step pressure-reducing approach. Using simulations with various valve opening modes, the viability of the system was proved. Robledo et al. [24] examined a microgrid integrated with HPV and all-electric dwellings. The results of a simulation of a year revealed that just above 70% of the yearly imported electricity could be decreased when the HPVs were run in V2G mode, leading to the net-zero-energy building goal. Li et al. [25] built an innovative algorithm for HPV economic estimation, proving the effectiveness of the algorithm using a number of cases for HPVs. Turgunboev and Saidov [26] confirmed the importance of hydrogen for the future development of vehicles. The major HPV components and battery electric vehicles were compared from the perspective of hydrogen

production and storage. Imanina et al. [27] introduced a model that could examine the impacts of typical factors on HPV acceptance. When using such a model, several factors which could affect HPV acceptance were examined.

Using evolutionary game theory and focusing on the present situation in China, Wang et al. [28] established the evolutionary partnership game model of the three participants (investment company, HPV user, and solar PV power plant). They also estimated the effects of some characteristic factors on the intentions of the three participants. The results showed stable states could be realized with various partnership modes. Higher solar intensity, longer annual sun duration, higher subsidies, and longer lifetimes of hydrogen charging facilities and PV panels were found to be preferred to smooth the partnership progress.

2.3 Biomass

The process of biomass gasification pertains to the transformation of organic substances, such as agricultural byproducts or specifically grown crops for energy production, into a synthesis gas (syngas) that comprises a blend of hydrogen and carbon monoxide. Subsequently, the aforementioned syngas has the potential to undergo additional processing procedures for the purpose of extracting hydrogen. Biomass gasification presents an ecologically sustainable method as it employs biodegradable refuse and can be deemed as having a carbon-neutral impact. Nevertheless, the procedure necessitates meticulous management and processing of the raw materials to prevent the discharge of noxious contaminants.

Biomass products have the potential for hydrogen production. Because of the high hydrogen content in biomass, it is therefore considered a promising renewable hydrogen resource [29]. Different types of biomass can be converted to hydrogen through various thermochemical and biochemical processes [30, 31]. Among such processes, supercritical water gasification (SCWG) is particularly attractive because of its adaptability to wet biomass. Under supercritical conditions of supercritical (temperature > 374°C and pressure > 22.1 MPa), water can hydrolyse low-reactivity macromolecules and participate in thermochemical reactions to produce H₂-rich syngas [32-34].

Currently, published works on biomass SCWG for hydrogen production concentrate mainly on the impacts of biomass properties and concentration, residence time, gasification temperature, reactor pressure, and reaction catalyst [35-37]. Optimal SCWG operating conditions may differ with feedstock properties and industrial aspects. Therefore, determining the optimum SCWG parameters in a particular case requires numerous experiments. However, the high temperature and pressure of SCWG make data collection challenging for the acquisition of experimental data [38]. The SCWG model is, therefore, more favorable.

2.4 Hydrogen Production Methods

Hydrogen has received considerable attention as a potential substitute for conventional fossil fuels, as the global community attempts to shift towards a more ecologically sound and renewable energy paradigm. In several industries, such as transportation and power generation for example, due to its high energy density and capacity to generate zero emissions when utilized as a fuel, hydrogen has gained significant interest. The production of hydrogen necessitates meticulous contemplation, as distinct techniques entail their respective benefits and obstacles. This section aims to examine and contrast various techniques for hydrogen production, emphasizing their viability and consequences for an environmentally responsible energy framework.

2.5 Steam Methane Reforming (SMR)

The prevalent technique for generating hydrogen is Steam Methane Reforming (SMR), which constitutes the bulk of the present worldwide production. The aforementioned procedure entails the reaction of natural gas with steam at elevated temperatures, resulting in the production of hydrogen and carbon dioxide. The utilization of natural gas, which is easily accessible, renders SMR a financially viable option. The emission of CO₂ can cause greenhouse gases release, unless measures such as carbon capture and storage technologies are used.

Steam Methane Reforming (SMR) is currently the leading technology for commercial and large-scale hydrogen production. Some studies have investigated mathematical models of catalytic tubular SMR reactors [39-42]. Models of steam reforming membrane reactors were developed by Giaconia et al. [43] (membrane steam reformers heated with molten salts), De Falco et al. [44-49] (2-D model of industrial membrane reactors), and Kyriakides et al. [50] (2-D model of a low-temperature membrane reactor). All the published works in this series focused on membrane reactors using packed bed catalysts. More recently, Bruni et al. have published other noteworthy studies on selective membrane integration. [51], Leonzio [52], and Kim et al. [53].

De Falco et al. [7] proposed a new model of the SMR process. They developed a novel solar steam methane reforming process for pure hydrogen production using molten salt heat transfer fluid, as shown in Fig. 1. The results revealed more than 3 Nm³/h of pure hydrogen production, reaching a total methane conversion of 60% at reactor temperature below 545 °C. A mathematical model of partial differential equations was solved by numerical simulation to investigate the influence of several operating conditions, such as the steam to carbon ratio, the sweep gas flow rate, and the molten salt inlet temperature. It was found that the simulation results were in good agreement with the experimental data with an average absolute error of < 2%.

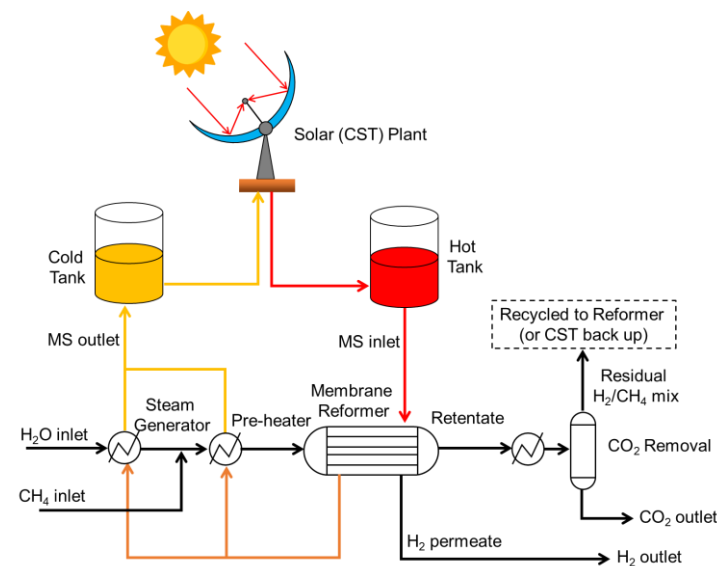


Fig. 1. Reformation of solar steam methane with molten salt heat transfer fluid for hydrogen production, reproduced from [7].

The utilization of offshore wind farms to produce hydrogen production has the potential to maximize the full capability of wind energy in the offshore, achieve decarbonization and energy security goals in electricity and other sectors, and overcome the constraints of grid expansion. The economic aspects of these systems are poorly understood. Dinh et al. [10] developed a novel integrated model for hydrogen produced from dedicated offshore wind farms as shown in Fig. 2. It was found that the discounted payback and net present value flowed for a number of storage scenarios were in good agreement with the viability model showing good results. The hydrogen production from the

dedicated offshore wind farm was also reported to be profitable in 2030 with the price of hydrogen sold at €5/kg. The storage capacities for underground storage were in the range of 2 and 45 days.

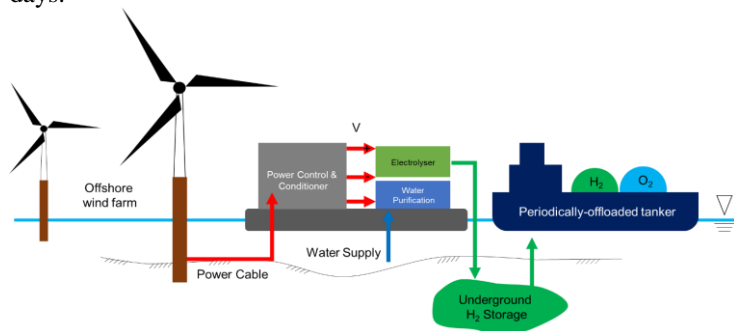


Fig. 2. A model of offshore wind farm viability assessment for hydrogen production, underground storage, and tanker transportation, reproduced from [10]

2.6 Electrolysis and Photoelectrochemical (PEC) Water Splitting

The utilization of electricity to dissociate water molecules into hydrogen and oxygen is a potentially advantageous technique known as electrolysis. The renewable energy utilization sources, such as solar or wind, can enable this process, resulting in a sustainable alternative. The process of electrolysis can be grouped into two categories, alkaline electrolysis and proton exchange membrane (PEM) electrolysis. The technology for alkaline electrolysis has reached a state of maturity and exhibits a high level of efficiency. On the other hand, PEM electrolysis presents faster response times and greater flexibility. The utilization of electrolysis as a primary technique for hydrogen generation holds significant promise, particularly in light of the increasing proliferation of sustainable energy sources.

The process of PEC water splitting involves the utilization of solar energy to facilitate the electrolysis of water, thereby leading to the direct production of hydrogen. The approach in question amalgamates the benefits of solar energy and electrolysis, thereby presenting a viable and effective solution from a sustainability standpoint. Notwithstanding the progress made in PEC water splitting, it remains at a nascent phase of development and encounters impediments with respect to scalability and cost-efficiency. Continued investigation and progress in technology exhibit potential for future utilization.

Overall, in light of the increasing demand for clean and sustainable energy sources, it is imperative to investigate diverse approaches to hydrogen production. The present article delineates that each method has its unique benefits, obstacles, and ramifications concerning sustainability. The process of Steam Methane Reforming is known for its cost-effectiveness; however, it necessitates the implementation of carbon capture measures to address its associated emissions. Electrolysis, particularly when energized by sustainable sources, offers a viable and eco-friendly alternative. Biomass gasification and photoelectrochemical water splitting are two promising methods for generating energy. The former involves the utilization of organic waste, while the latter is a solar-driven process. In conclusion, the integration of various techniques and continual progress in technology will facilitate the establishment of a varied and ecologically conscious hydrogen production infrastructure, thereby bolstering the worldwide shift towards a more sanitary and enduring energy prospect.

2.7 Battery Electric Vehicles (BEV)

Electric vehicles are considered a promising technology for the future [54, 55]. Normally, the studies of economic development, carbon emission, and energy consumption have been investigated separately in the literature. Awodumi et al. [56] examined the role of nonrenewable energy consumption in carbon emissions in

Africa, showing evidence of the asymmetric impact per capita of natural gas and petroleum consumption on economic growth and carbon emission. Furthermore, Waheed et al. [56] carried out a survey on economic growth, energy consumption, and carbon emissions for developing and developed countries. It was reported that high energy consumption was the main cause of carbon emissions. Ahmadi [57] suggested the use of electric vehicles for decarbonization in the sector. Their results revealed that both plug-in and fuel-cell electric vehicles showed improved air quality represented by emission reduction as opposed to conventional internal combustion engines. Note that hydrogen infrastructure and its reliability are critical for such a realization in the transport sector [58].

Although several studies on economic growth, carbon emissions, and energy consumption are available [59-62], a comprehensive study that incorporates the causes, trends, and solutions of carbon emissions is difficult to find. Bamisile et al. [63] proposed a comprehensive approach to solving future carbon emissions by focusing their study on Africa. To determine the relationship between carbon emission and economic development, 25 African countries from five African geopolitical zones were selected. In all sectors, carbon emissions and gross national income were found to be significantly positively interrelated. With the increasing national wealth in Africa, carbon emissions also increased in the continent. The total annual CO₂ emission was projected to increase by 2022 compared to 2018 as shown in Fig. 3. The use of renewable energy technologies in the power industry plays an important role in decreasing CO₂ emission. However, the incorporation of hydrogen production and battery electric vehicles is the key to fully maximising electricity generation from renewable energy sources.

2.8 Artificial intelligence method

Artificial intelligence, including machine learning (ML), has attracted considerable attention owing to the rapid progress in this field. Several algorithms such as Support Vector Regression [64], Artificial Neural Networks [65], Adaptive Network Based Fuzzy Inference System (ANFIS) [66], and Prophet [67] have been extensively used, including in finance [68], energy [69], load management [70], diseases [71], and weather [72].

A machine learning model functions as a practical instrument for precisely predicting hydrogen generation. Through the examination of extensive historical data and the identification of patterns and correlations, the model has the capability to generate dependable forecasts regarding forthcoming hydrogen production quantities. The model incorporates multiple variables, including energy consumption, meteorological patterns, sustainable energy resources, and manufacturing facilities. The system employs sophisticated algorithms and statistical methodologies to effectively handle and examine the data, thereby facilitating the provision of significant observations pertaining to the trends in hydrogen production.

By utilizing a machine learning algorithm, stakeholders within the hydrogen sector can effectively make informed decisions and optimize their production processes. The forecasting abilities of the model enable it to predict variations in the demand for hydrogen and make necessary modifications to the levels of production. This practice guarantees optimal allocation of resources, minimization of waste, and maximization of profitability. Moreover, the model's capacity to take into account extraneous variables such as meteorological conditions empower operators to enhance the utilization of renewable energy for hydrogen generation, culminating in a more environmentally sustainable and ecologically conscious approach. In essence, the utilization of a machine learning model as a predictive instrument provides the hydrogen sector with the ability to engage in strategic planning and satisfy the increasing need for sustainable energy.

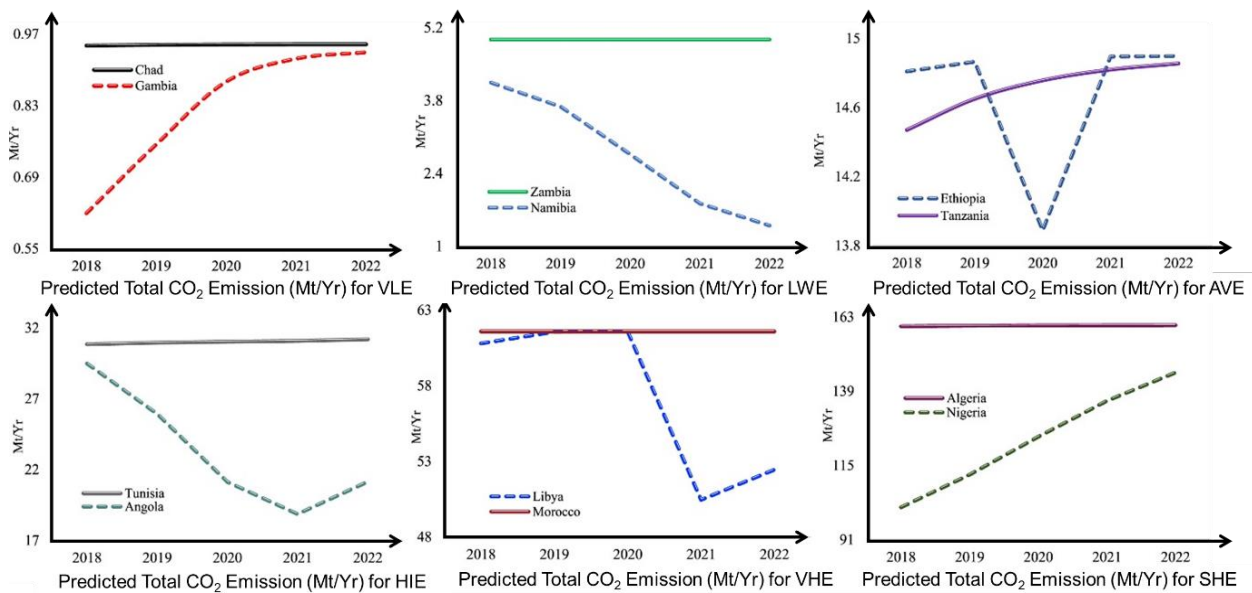


Fig. 3. Projection of total CO₂ emissions from 2018 to 2022 for various African countries, reproduced from [63].

A machine learning model is a practical tool for forecasting hydrogen production. It can clarify the effect of some variables involved in SCWG, being useful in choosing the suitable feedstock and optimizing a number of parameters in the real experiment. Haider et al. [73] used Machine Learning to predict solar hydrogen production in Islamabad, Pakistan. A photovoltaic-electrical system was selected to predict electricity and, thus, hydrogen production. The weather data used had been recorded for 13 and a half months using accurate meteorological instruments (Fig. 4). Three different algorithms were evaluated: Stochastic Gradient Descent, Prophet, and SARIMIX. Prophet showed the best performance with 3.7% of the mean absolute percentage error, predicting a daily average hydrogen production of 93.3×10^3 kg/km², indicating a great potential for solar hydrogen production in Islamabad, Pakistan.

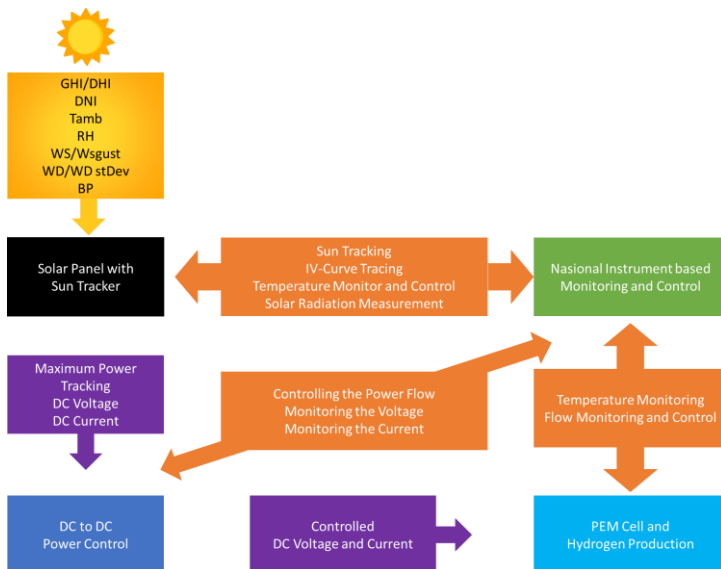


Fig. 4. Forecast of the Islamabad hydrogen production potential from solar energy using water electrolysis, reproduced from [73].

The use of SCWG of biomass to produce hydrogen is a time-consuming and expensive process. It is important to develop an accurate model for SCWG process prediction and evaluation. Zhao et al. [4] introduced four machine learning models to forecast hydrogen production through biomass SCWG, interpreted the inner workings of the optimal model, and evaluated the performance of SCWG. It was found that the random forest model gave the best performance in predicting hydrogen yield with an R²

of 0.9782). The contour plots according to the RF model revealed that the highest hydrogen reaction efficiency of 45.6% and the exergy efficiency of 43.3% were achieved using biomass with a high O content and low H/C ratio as the feedstock.

3 Conclusions.

In conclusion, the current dominance of petrol fossil fuels and small-scale water electrolysis in hydrogen production highlights the need for a shift towards renewable hydrogen sources. It is crucial to replace fossil-derived hydrogen with renewable alternatives. Once hydrogen production processes are further developed and matured, they can serve as viable fuels for both combustion burners and vehicle engines. Full commercialization of fuel cell technology will be paving the way for hydrogen to be utilized as fuel in fuel-cell electric vehicles. To address the challenges in the renewable energy sector, it is imperative to consider fair energy pricing and implement a carbon trading or tax structure that holds polluters accountable by factoring in the cost of CO₂ emissions. Additionally, an intriguing approach would be to establish a carbon-to-hydrogen endowment model, where carbon-producing entities contribute to the development of a hydrogen economy. This model could play a pivotal role in overcoming obstacles and fostering the growth of renewable energy sources. By emphasizing the urgency of transitioning to renewable hydrogen and proposing concrete strategies for its integration into various sectors, we can propel the advancement of sustainable energy solutions and pave the way for a greener future.

4. Future Recommendation

Based on the outcomes and deductions delineated in this investigation, there exist a number of suggestions for forthcoming research endeavours that could augment our comprehension and application of hydrogen as a substitute energy resource.

1. The advancement of technology requires persistent research and development efforts that prioritize the enhancement of efficiency and cost-effectiveness of hydrogen production methods. This can be achieved through the exploration of novel catalyst materials and optimization of electrolysis processes. The practicality and widespread adoption of hydrogen as an energy carrier can be significantly enhanced by advancements in storage technologies, such as materials designed for high-density hydrogen storage.

2. The development of infrastructure is crucial for the successful integration of hydrogen into current energy systems. In order to achieve this, it is imperative to conduct additional research to evaluate and create the essential infrastructure components, including hydrogen refueling stations, pipelines, and distribution networks. The assessment of the viability, expandability, and security considerations of said infrastructure will be pivotal in the triumphant implementation of hydrogen-centered technologies.
3. Undertaking thorough life cycle assessments (LCA) can yield significant insights into the ecological ramifications linked to the complete hydrogen production process. Prospective research endeavors ought to prioritize the assessment of the environmental and energy efficiency throughout the life cycle of diverse hydrogen production routes, while considering variables such as resource utilization, discharges, and refuse generation.
4. The analysis and development of efficient policy frameworks and market strategies can facilitate the expeditious transition towards a hydrogen-based economy. Subsequent research endeavors ought to investigate the efficacy of policy incentives, regulations, and financial mechanisms in facilitating the uptake of hydrogen technologies and fostering the expansion of a thriving hydrogen market.
5. The exploration of the interdependent relationship between hydrogen and other renewable energy sources, such as solar and wind power, is crucial in establishing a cohesive and enduring energy infrastructure. Prospective investigations ought to examine novel approaches to incorporate hydrogen production with sporadic renewable energy generation, such as utilizing surplus renewable electricity for electrolysis or investigating power-to-gas conversion technologies.
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By exploring these prospective research domains, it is possible to enhance the potential of hydrogen as an environmentally friendly and sustainable energy alternative and expedite the shift towards a low-emission future.

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