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Innovations and Challenges in Water Electrolysis for Sustainable Hydrogen Production

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Abstract: Hydrogen is renewable, efficient energy carrier that can contribute to solve the climate change problem when paired with sustainable electricity and water electrolysis. While PEM electrolysis is outstanding in producing high purity of hydrogen, the AWE electrolysis has been Versatile in meeting several industrial purposes. AEM technology is considered as more cost effective than the existing technologies which uses highly costly metal catalysts such as Pt, Au, Ru, etc.

However, water electrolysis which is a sustainable method for hydrogen production supplies only 4% of the global hydrogen due to high costs. Unfortunately, the use of precious metals constrains the prospect of scale-up; nevertheless, automation-based naked-metal electrocatalysts can be advanced as cost-effective yet conductive and electrocatalytically active solutions. But much more work has to be done to improve their characteristics and stability.

In the context of this paper, the major developments and problems in water electrolysis are discussed based on the outlook for the effective and inexpensive catalysts for hydrogen and oxygen evolution reactions. To this end, it seeks to overcome these barriers in order to provide direction to future studies and facilitate the development of cost-effective water electrolyzers for sustainable hydrogen generation.

Keywords: Hydrogen Production, Water Electrolysis, Hydrogen Evolution Reaction (HER), Oxygen Evolution Reaction (OER), Renewable Energy.

1. INTRODUCTION

These conventional resources include fossil and nuclear energy in their use results in environmental problems like wastes, pollutant emissions, climate change, and depletive of resources hence call for sustainable sources [1] . As standards of living and global population continues to increase, the demand for energy increases thereby leading to the craze for renewable energy such as hydrogen. While hydrogen is a carbon-free energy carrier with the largest energy density of 140 MJ/kg, it goes beyond traditional fuels [2].Non-renewable energy source usability was amounting to 1230 GW in the year 2009; the growth rates in wind energy to 38GW and hydropower systems to 31 GW ; [3].In clean production methods, water electrolysis is distinguished for generating pure hydrogen and oxygen but accounts for only 4% hydrogen generation worldwide because the cost for the electrocatalyst is high [4].. [5] Ruthenium and platinum compounds found effective in the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) but expensive and rare and therefore requires NNPMs. Electrolysis of water into hydrogen and oxygen requires highly corrosion resistant and catalytically active anode and cathode; the technology poses safety and durability issues [6].Higher temperatures favor the electrochemical activity of the electrolyte and the kinetics at the electrodes; however, these conditions are accompanied by increased corrosion rates due to the effects of pH fluctuations and air quality [7]. Mitigating these challenges is crucial to the improvement of water electrolysis as one of the hydrogen production technologies.

Hydrogen Production Sources	Percentage of Global Hydrogen Production	Share (%)	Method	Volume Bcm3/year	References
Natural Gas	75	48	Steam Methane Reforming, SMR	240	(Dash et al., 2023)
Coal	2	18	Coal Gasification	90	(Wagner et al., 2008)
Wind	Hoped to be contribute	-	Wind-Electrolysis	-	(Correa et al., 2022)
Nuclear	Hoped to be contribute	-	High-Temperature Nuclear Heat	-	(Elder & Allen, 2009)
Oil	30	30	Steam Methane Reforming (SMR)	150	(Bhat & Sadhukhan, 2009)
Solar	Hoped to be contribute	-	Photovoltaic-Electrolysis (PV-E)	-	(Grimm et al., 2020)
Biomass	3	-	Biomass Gasification	-	(Molino et al., 2016)
Water (Electrolysis)	65	4	High-temperature, high-pressure electrolysis	20	(Ganley, 2009)

Table 1: - Hydrogen Production Sources

The table reviews hydrogen production techniques with the focuses on water electrolysis and steam methane reforming, in which currently 75% of hydrogen globally is produced using natural gas [8]. Coal gasification and high-temperature nuclear energy are expected to account for major shares and contribute 2% of volume hydrogen volume and 90% hydrogen volume respectively. [9]. There is a critical contribution as follows: SMR of oil 30% = 150 Bcm per year Hydrogen production from biomass gasification is 1 to 3%.

In 2050 it is anticipated that water electrolysis would be framing 65% of the world's hydrogen outturn, which is valued to be of 20 cubic meters annually [10]. Nevertheless, the fact is that electrolyzes are sensitive to water quality because contamination may affect the efficiency, durability, and hydrogen purity. The present document discusses fundamental and advanced aspects of the water electrolysis process along with the design, performance analysis, and future trends for researchers in the field to consider for the commercialization.

2. RELATED WORKS

2. Fundamentals of Water Electrolysis

2.1. Basic Principles and Mechanisms of Water Electrolysis:

Water electrolysis, a sustainable method for small-scale energy production, conversion, storage, and use in remote communities, uses renewable electricity to generate hydrogen for heating and energy storage. Hydrogen can be produced from excess renewable energy sources by electrolyzing water, which can be used to produce fuel gas or electricity in fuel cells. [11].

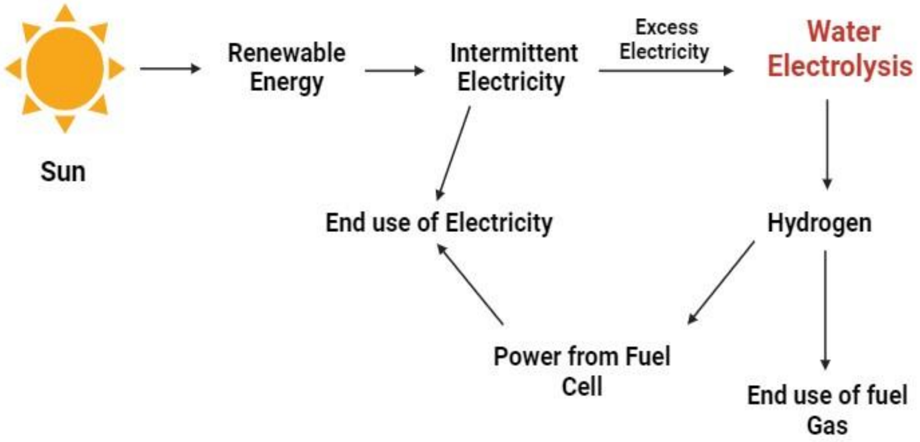

Figure.1. A schematic illustration of a hypothetical distributed energy system where water electrolysis plays a major role in the production of hydrogen, a fuel gas, and an energy storage mechanism.

Water electrolysis is a process where water molecules are split into hydrogen and oxygen gasses through an electrochemical process. Water electrolysis is a process that separates hydrogen and oxygen into gaseous stages, generating clean energy without causing pollution from power usage. [12].

$$H_2\ (g) + \frac{1}{2}\ O_2\ (g) = \text{Energy} + H_2O\ (\text{Liquid}) \quad \text{---------------------} \quad (1)$$

Electrical energy from a DC power source is needed for water electrolysis. When the temperature is room temperature, there is relatively little water splitting roughly 10^{-7} moles/liter because to the extremely low cost of pure water electricity. Acid or base is used to enhance conductivity in alkaline electrolyzes, where water is combined with KOH, NaOH, and H_2SO_4. This creates positive and negative ions, which easily conduct electricity.

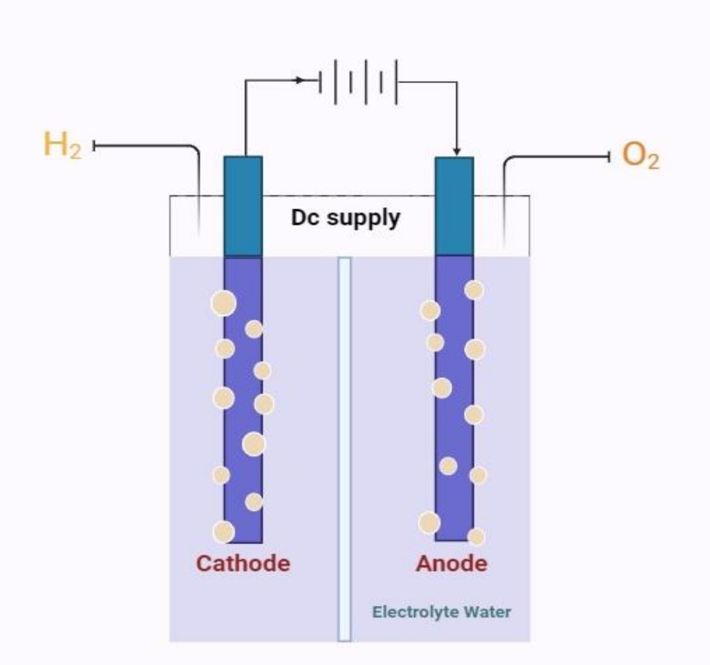

Figure.2. the basic steps involved in the electrolysis of water.

Figure 2 illustrates the basic concept of an electrolysis cell, which operates on the same principle: hydrogen and oxygen gas bubbles form at the cathode and anode of an electrochemical cell when high voltage is applied. [13].

2.2 Description of the Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER):

Water splitting for hydrogen production involves electrocatalytic reactions: HER and OER. The efficiency can be predicted with regard to electrocatalyst as well as the selected electrolyte system. In modern systems, understanding the relationships existing between the structure and properties of the electrocatalysts is essential in system advancement [14]. Electrolytic cell is made up of an anode a cathode and an electrolyte in between. HER turns water into hydrogen then OER forms oxygen. OER has lower reaction rate showing formation of OH groups and protons during water dissociation [14].|

2.3. Factors Influencing the Kinetics and Efficiency of Electrolysis Reactions:

2.3.1: Electrode Material:

Catalyst type influences diffusion characteristics of the reaction based on electrode conductivity, where highly conductive metals like platinum yield faster electron-transfer rates and exhibit low resistive losses. The electrochemical properties of the catalyst include aspect ratio, chemical resistance, and catalytic performance for long-term stability and performance. All costs, the needs of the applications, and compatibility of electrolytes are determining factors for material choices [15].

2.3.2 Electrolyte Composition

Contrary to their formal names suggesting they facilitate the movement of ions, which help control reaction rates. Increasing the ionic conductivity and optimizing the pH as well as the efficiency of additives particularly sulfuric acid as well as improving proton transport and selectivity increases efficiency [16]

2.3.3 Temperature

Higher temperatures improve ionizer conductivity of the solution and decreases the activation energy therefore promoting fast reactions rates (Arrhenius equation) . However, high temperature poses challenges of electrode and electrolyte values and therefore, temperature regulation is important [17].

2.3.4 Current Density

Density of the current that pass through the electrolyte and cross-section area of the electrodes is the two factors that affect efficiency of electrolysis. High density can result in higher over potential thereby deteriorating the performance. Faraday’s law measures the amount of substance that is produced in an electrolysis process. Current density is improved by choosing materials and electrolytes [16].

2.3.5 Pressure

Several factors cause pressure to have an impact where solubility of gas, mass transfer rates, and reaction rates is concerned. High pressures belong to the operating conditions which positively influence the efficiency of PEM electrolyzer due to better flow characteristics of the gases and losses. More work can still be conducted to improve pressure levels in order to enhance results [18].

3. METHODOLOGY

3. Challenges in Water Electrolysis:

3.1 Slow Kinetics Due to the Low Conductivity of Water

3.1.1: Impact of Low Water Conductivity on Electrolysis Kinetics:

3.1.1 .1. Slower Ion Transport:

Low water conductivity of the medium restricts the movement of ions that participate in a reaction and accordingly reduces efficiency. These include formation of bubbles on the electrodes and low ion density as constraints in its performance [19]. Improvement of proton conductivity is the key factor to increase the reaction kinetically.

3.1.1 .2. Increased Ohmic Resistance:

High resistance occurs because of low conductivity which in turn hampers efficiency in oxygen evolution reactions [20]; This is further complicated by gas bubbles which distort the resistance through hampering ion flow.

3.1.1 3. Limited Reaction Sites:

Low ionic conductivity limits the number of active sites for the reaction on the electrodes and hence limits hydrogen and oxygen formations. These limitations are However, electrode conductivity, electrolyte concentration, and temperature optimization can help solve these.

3.1.2 Strategies to Enhance Electrolysis Kinetics in Low-Conductivity Water:

3.1.2 1. Electrode Design and Material Selection:

The electrochemical performance and reaction kinetics can be enhanced by altering properties of electrodes, for instance, nano structured coatings, and suitable choice of electrolytes [21].

3.1.2 2. Additives and Doping:

Catalytic materials are then improved by the addition, doping, or structural alteration, to improve conductivity and decrease overpotential.

3.1.2 3. Temperature and Pressure Adjustments:

Elevated temperatures reduce the preference for ion movement while high pressure improves the occurrence of reaction events in low conductivity water [22]**.**

3.1.2 4. Pulsed Electrolysis:

Pulsing the voltage or current decreases energy consumption and increases productivity especially in low conductivity conditions [23].

3.2 Chlorine Evolution Reaction (CER) and Corrosion

During electrolysis CER building results in electrode corrosion and chlorine species emission (such as Cl_2, Cl_2O, ClO_2) which are operation issues. The Ehrenburg mechanism and the mixed oxide electrodes have enhanced catalytic features, which eliminates issues such as stray currents and the formation of destructive corrosion [24].

3.3 Thermodynamic Stability of Water: Need for Overpotential

Water's thermodynamic stability requires overcoming an overpotential to initiate electrolysis. High-temperature electrolysis (e.g., ~1000°C) reduces energy consumption but necessitates advanced materials like super-alloy nanowire catalysts and optimized electrode designs [25].

3.4 pH Variation during HER and OER

The water electrolysis process, which uses an electric current to split water molecules into hydrogen and oxygen, produces hydrogen when the authorized renewable energy sources are used to power it. Following its production, hydrogen can be stored, transported, and utilized to make other fuels [26]. Even though the OER has been studied at a variety of pH values, a mechanistic understanding of how it functions remains lacking, especially in circumstances when the pH is not high. For acidic and alkaline conditions, respectively, the OER is shown in equations 1 and 2.

$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$

$4e^- + 2H_2O + O_2 \rightarrow 4HO^-$

Catalyst nanoparticles, including films and single or polycrystalline forms, have been examined half-cell (rotating disk electrode) and full cell (membrane electrode) to evaluate the oxygen evolution reaction (OER) in electrical and photo-electral circuits [27]. . Hydrogen formation in the course of metal electroplating in acidic solutions tends to be attributed to changes in pH values at an interface. This is experienced during the electrodeposition of Co, Zn, Fe, ZnFeCoW, ZnCo, ZnNiCoFe, NiCoFe, and FeNi [28]. For these cathodic polarization studies, the value is often high enough to initiate the hydrogen-evolution reaction, effectively concentrating the phosphate or other buffer at the electrode/electrolyte boundary, even in relatively buffered electrolyte solution [29]. The HER mechanism is strongly influenced by environmental conditions, involving three key steps in acidic media: the Volmer step (1a) that forms adsorbed hydrogen [30], then either the Heyrovsky step (1b) and or the Tafel step (1c) to produce H2.

$H_{ad} = H^+ + e^-, \qquad (1a)$

$H_2 = H_{ad} + H^+ + e^-, \qquad (1b)$

$H_2 = 2H_{ad}. \qquad (1c)$

Concerning the alkalinity induced HER response in media. The two possible reaction steps are the Volmer step (2a) and the Heyrovsky step (2b), as shown by the matching equations below:

$H_{ad} + OH^- = H_2O + e^-, \qquad (2a)$

$H_2 + OH^- = H_{ad} + H_2O + e^-. \qquad (2b)$

In alkaline conditions, water dissociation, hydroxy adsorption (OH_{ad}), and trade-off of Had are necessary to sustain HER activity. Theoretical simulations indicated a relationship between HER activity and hydrogen adsorption (H_{ad}). The free energy of hydrogen adsorption (ΔG_H) is a widely recognized characteristic of a hydrogen evolution material [31].

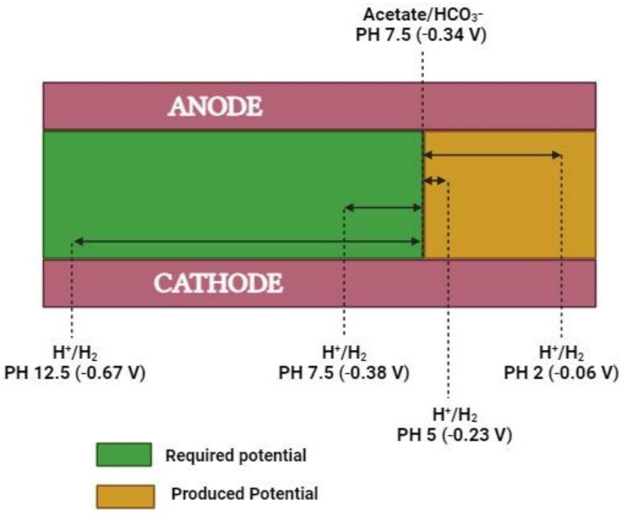

Figure 3: Hydrogen Production using a pH Control Strategy

Therefore, the purpose of this research is to determine whether a two-chamber MEC's performance may be enhanced by adding pH control to the anodic and/or cathodic chambers. The benefits of operating at a low pH at the cathode will also be assessed using two different methods:

(i) raising the current intensity and maintaining a high applied potential (1.0 V) to boost hydrogen production, and
(ii) Lowering the applied potential significantly while maintaining the same level of hydrogen production [32].

Experiment Number	Anodic pH control	Cathodic pH control	Agitation	Potential applied (V)
E1	Not controlled	Not controlled	No	1.0
E2	Not controlled	7.5	Yes	1.0
E3	7.5	Not controlled	Yes	1.0
E4	7.5	7.5	Yes	1.0
E5	7.5	2.0	Yes	1.0
E6	7.5	5.0	Yes	1.0
E7	7.5	12.5	Yes	1.0
E8	7.5	2.0	Yes	0.2

Table 2. An overview of the experimental setup for batch experiments E1 through E8

The experiments conducted for this inquiry are summarized in **Table 1.** Here are a handful of these: A series of experiments (E4, E5, E6, and E7) with the cathodic pH controlled at different values; (iv) a batch experiment with a low cathodic pH (2.0) and low applied potential (0.2 V; E8); (ii) batch experiments with pH control solely in the cathodic (E2) or anodic chamber (E3) [33].

4. RESULTS AND DISCUSSION

4. Technological Approaches and Solutions

4.1 Overview of Advanced Materials, Catalysts, and Electrolysis Cell Designs

4.1. 1. Advanced Materials:

Scientists are developing efficient materials with high catalytic activity, longevity, and better conductivity for electrodes, including transition metal oxides, carbon-based, and metal alloys. These materials enhance reaction kinetics, reduce electrode corrosion, and offer promising alternatives to conventional bioelectrochemical systems. Single atom-catalyzed materials are also being explored for advanced energy storage [34]. Bimetallic hybrid catalytic materials, such as Pd-Ir nanoparticles, show potential applications in chemical reactions involving α, β-unsaturated acids and esters, offering higher electrocatalytic performance and durability, [35]. Lori explores ceramic Hippocratic rings' benefits in polymer electrolyte fuel cells, highlighting their durability and enhanced metallic catalyst performance, promoting the development of materials with high catalytic activity.

4.1.2 Catalysts

Catalysts added to a reaction decreases the activation energy and hence increases the rate of the reaction. Platinum is relatively popular, but since it is expensive, its utilization on a large scale is impossible. Non-Precious Metals: Exb ranks of nickel, iron and cobalt show almost the same efficiency as platinum-group metals and at very low cost. Duplicate enzymatic pathways to mimic transition states in order to optimize the use of enzymatic reactions in the catalytic activity [36].

4.1. 3. Electrolysis Cell Designs:

Innovative electrolytic cell designs aim to enhance efficiency and performance by developing large surface areas, active ions transport mass, and energy losses. These designs include flow-through electrodes, porous structure electrodes, and membrane-electrode assemblies, paving the way for next-generation electrolysers. Innovative electrolytic cell designs aim to enhance efficiency and performance by developing large surface areas, active ions transport mass, and energy losses. These designs include flow-through electrodes, porous structure electrodes, and membrane-electrode assemblies, paving the way for next-generation electrolysers [37].

4.2 Case Studies: Best Practices of New Electrolysis Technologies

4.2. 1. Alkaline Electrolysis:

Alkaline electrolysis, a large-scale hydrogen production process, has shown efficiency and cost-effectiveness in renewable energy projects. Recent advancements include room temperature water electrolysis with an alkaline polymer electrolyte and non-noble catalysts, and a long-life, high-performing alkaline membrane water electrolysis system using an anion exchange membrane and an ionomer for hydroxide conductivity [38]. López-Fernández's research paper discusses advancements in water electrolysis for alkaline exchange membrane, indicating that with further efficiency and scalability improvements, it can be successfully implemented.

4.2. 2. Proton Exchange Membrane (PEM) Electrolysis:

Lately, the water splitting through the PEM technology has resulted in groundbreaking discoveries that make these advancements well placed in the energy sector. The efficiency of the MEAs designed by Kim (2018) and Siracusano was evaluated in continuous water electrolysis experiments where their MEA's showed similar or slightly lower performance to the commercial Nafion-based MEA [39]. In addition, Millet presented the GenHyPEM project, a software package developed to optimize the performance of a PEM water electrolyze, and electrochemistry which have allowed the use of non-noble electrocatalysts. Smolinka described the technical process of PEM water electrolysis and how the material was used to enhance energy conversion, performance and production rate. The studies jointly exemplify the potential of PEM electrolyze in water electrolysis.

4.2.3 High-Temperature Electrolysis

High-temperature electrolysis uses solid oxide electrolytic cells for efficient and thermal waste utilization. Successful examples show integration with industrial applications, co-generation plants, and renewable sources. Plasma heat electrolysers for water electrolysis show remarkable results, with Dönitz's observation demonstrating high current density and Faraday efficiency. Nikiforov highlighted the development of non-platinum catalysts to reduce costs, while Salzano's high temperature-electrolysis can increase energy efficiency by 1000 times. [40]. These studies demonstration the fact that temperature water electrolysis is promising and can be successful under any conditions.

4. 3. Comparisons between Seawater Electrolysis and Pure Water Electrolysis:

4. 3. 1. Product Cost:

In spite of the fact that seawater electrolysis has challenges, such technology is evaluated as the most cost-effective compared to water electrolysis due to the large-scale seawater availability. Nevertheless, Kibria2021 and Khan2021 claim that the financial and environmental rewards of seawater electrolysis are not so big, with the former asserting that the immediate shifting of investments is inevitable. Fesenko on the prudential shelving of natural water direct electrolysis and efficiency also illustrated the prospect of seawater electrolysis cost effectiveness.

4. 3.2. Energy Consumption:

In seawater electrolysis studies, it has been demonstrated that it is a viable means of hydrogen production and in particular it is effective in regions with limited clean water access. Regarding this matter, oxygen evolution reaction kinetics is slow, chlorine evolution reactions are occurring simultaneously which are bad for the battery and chloride ions decompose the electrode. Nevertheless, seawater electrolysis could be a more efficient method compared to the traditional pure water electrolysis, and this can be much more applied when renewable energy is considered.

4. 3.3. Environmental Impact:

Seawater electrolysis for hydrogen production is an emerging process, which is also facing some problems, namely slow kinetics, competing reactions, and electrode degradation. While this approach comes with many challenges, it still shows comparable environmental impact to pure water electrolysis and its adoption does not significantly raise the financial cost nor the CO2 emissions. Notwithstanding that, the water sources availability, condition, and cost will influence the applicability as is the seawater. On account of it, while seawater electrolysis is promising, more research is demanded to find technical solutions and also to evaluate its natural environment impacts in different situations.

Discussion

5. Current Research and Future Directions of Hydrogen Production from Sea Water

5.1. Review of Ongoing Research Efforts Aimed at Overcoming Challenges in Water Electrolysis.

The interest in the production of hydrogen from seawater has given rise to multiple research projects that tackle the technical issues that hinder water electrolysis [41]. Seawater hydrogen generation has significant potential for sustainable energy production. Researchers are exploring methods like seawater electrolysis, photoelectrochemical cells, and microbial electrolysis to extract hydrogen efficiently. The primary goal is to develop cheap, environmentally friendly hydrogen production technologies at an industrial scale. Key issues include improving electrolysis efficiency and using more efficient catalysts.

5.2. Recommendations for Future Research Directions and Technology Development

In order to effectively explore the potential of hydrogen production from sea water, the following recommendations for future research directions and technology development can be considered:1 [42]. Research should focus on developing efficient catalyst materials for seawater electrochemical splitting to produce hydrogen. High-efficiency electrolysis methods should be optimized, and overall energy conversion efficiency should be improved.

6. Integration with Renewable Energy Sources

As for the source, seawater can be regarded as a perspective candidate for the hydrogen production that is compatible with renewable power sources like PV and wind energy ones. These renewable resources supply the electrical power for the water decomposition process making certain sustainable and constant hydrogen generation. Because it harnesses excess electricity produced by renewables when demand is low, seawater electrolysis fills the energy gap appropriately and does not waste energy. This process integrates hydrogen energy, synthetic fuels and sea water distillation and the result is a cheap track to renewable energy [43] . Furthermore, the energy reserved as hydrogen during the process of electrolysis initiates the flow of variability in renewable energy and contributes to the reliability of using renewable energy products in today's society. Hydrogen production from seawater reduces emission of greenhouse gases during the process and supports ability to store carbon, thus drawing positive nods from the environmentalists [44].

5. CONCLUSION

The increasing need of clean energy can be effectively solved by adopting water electrolysis which involves the extraction of hydrogen from seawater. Combined with renewable power like solar and wind, seawater electrolysis offers a stable and virtually unlimited supply of hydrogen. Though, problems like poor oxygen evolution reaction kinetics, chlorine evolution, electrode degradation and formation of cathode precipitate still remain. New solutions towards solving these problems include improvement of electrodes and electrolyzes. Further studies are required to fine-tune energy application and consumption, cost, and emission rates. Continuous seawater hydrogen production enhances the generation of a cleaner economy since it does not rely on fossil fuel sources while it is useful in many sectors including transport, energy storage, and manufacturing. New developments in the field of electrolysis technology and viable catalysts may lead towards even greater efficiency and cost cutting of hydrogen production, which is vital for sustainable hydrogen economy future.

Due to increased generation of renewable energy sources, seawater electrolysis can assist in the construction of the low-carbon economy for the use of hydrogen in an ecological outlook.

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