# Multi-scale Structural Characteristics and Efficiency Analysis of Proton Exchange Membrane Water Electrolysis Hydrogen Production Technology

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**Abstract.** Driven by the global energy transition and carbon neutrality goals, proton exchange membrane water electrolysis (PEMWE) technology has become the core technology for large-scale hydrogen production due to its advantages of high efficiency (74%-87%), fast response (millisecond level), and high-purity hydrogen production (99.999%). However, the industrialization process is limited by key bottlenecks such as the high cost of precious metal catalysts, the high cost of titanium-based bipolar plates, and the system investment cost. Based on the multi-scale analysis framework, we proposed a gradient catalytic layer design to reduce the precious metal load by 30%-50%, an ultra-thin proton exchange membrane (<50 μ m) to optimize the mechanical and chemical stability, and a three-dimensional corrugated flow field structure to reduce the two-phase flow resistance by 20%-35% and improve the current density uniformity by 40%. The research results provide a theoretical basis and technical solution for breaking through the cost and efficiency bottleneck of PEMWE technology, and promote its large-scale commercial application.

## 1 Introduction

Under the current global energy transition situation, the unsustainability of the fossil energy consumption structure becomes more conspicuous. With a high calorific value (120 MJ/kg) and zero carbon emissions at the terminal application, the technologies that are able to produce large-scale hydrogen energy have become a key research direction in the energy revolution. Among various hydrogen production technologies, proton exchange membrane water electrolysis (PEMWE) technology demonstrates its significant advantages with its unique multiphase transport mechanisms and electrochemical kinetics, for instance, the nanostructured catalytic layer of the membrane electrode assembly (MEA) [1]. The system's energy transformation efficiency ranges from 74% to 87%, which is significantly better than

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alkaline electrolysis technology [2]. The hydrogen that it produces has a purity of 99.999% (by volume), meeting the needs of fuel cell applications. Moreover, with millisecond-level dynamic response, it can naturally fit the fluctuating power supply of renewable energy.

However, the industrialization of this is inhibited by the "structure-performance-cost" paradox of its key material systems. At the mesoscale, the loading of precious metal catalysts (Ir/Ru-based) must be maintained at 1-2 mg/cm$^2$ [3]. At the macro component level, the optimization of the flow field structure and surface modification processes of titanium-based bipolar plates accounts for 48% of the total electrolyzer cost [4]. The structural contradictions of this material system lead to the current unit investment cost of PEM electrolyzers (approximately $1200/kw) remaining 3-4 times higher than that of traditional alkaline technology, limiting PEM technology's hydrgen production to only accounting for 4% of global hydrgen production [5,6].

This paper systematically interprets the coupled effects of key structural parameters, such as proton conduction networks, gas-liquid transport channels, and current distribution uniformity on overall performance in PEMWE technology, by constructing a multi-scale analysis framework spanning "material microstructure, component mesostructure, and system macrostructure". It focuses on engineering pathways for reducing noble metal usage through gradient-structured catalyst layer design, strategies for enhancing the mechanical and chemical stability of ultrathin proton exchange membranes (<50 μ m), and the regulation mechanisms of three-dimensional corrugated flow field structures on two-phase flow resistance and current density distribution. The conclusion of research provides theoretical insights and technical optimization pathways to overcome the cost barriers and efficiency limitations of PEM electrolysis technology.

## 2 The principle of PEMWE technology

PEMWE is an advanced technology that produces high-purity hydrogen by the electrolysis of water. Its fundamental principle involves applying a direct current power source across the PEMWE cell to promote the decomposition of deionized water into hydrgen and oxygen, which converts the electrical energy into the chemical energy of hydrgen. The core of PEMWE technology is the PEMWE cell, which is structured from the inside out as follows: proton exchange membrane, porous transport layer, and bipolar plates.

In the anode chamber, deionized water enters the porous transport layer through flow channels. After dispersing into microdroplets, the water loses electrons and releases hydrgen ions and oxygen because of the oxidation at the anode catalytic layer. Then the oxygen is emitted through the flow channels. Meanwhile, the hydrgen ions migrate across the proton exchange membrane to the cathode catalytic layer under electrostatic attraction. After that, the hydrgen ions gain electrons and become hydrgen gas, which is also expelled through the flow channel [7]. The working principle of PEMWE is demonstrated in Fig. 1 [8].

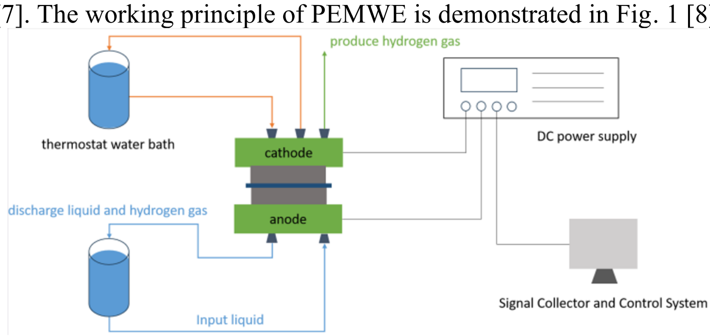


**Fig.1.** The working principle of PEMWE [8].

The proton exchange membrane (PEM) has selective permeability, allowing hydrgen ions to pass through and hindering other ions effectively. Right now, perfluorosulfonic acid membranes are the main type of proton exchange membrane, which has high durability with a typical service life of up to 10000 hours. It is also equipped with fantastic electrical conductivity, featuring a proton conductivity of over 0.1 S/cm [9].

The membrane electrode assembly (MEA) constitutes a core component in both PEM water electrolysis and anion exchange membrane water electrolysis. Its structure encompasses an ion exchange membrane along with a pair of electrodes dedicated to the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). These electrodes are fabricated from catalysts and support materials. The performance and stability of the catalyst coating can be significantly enhanced by optimizing the catalyst layer thickness, improving coating uniformity, utilizing novel membrane materials, and refining manufacturing processes [10]. In practical preparation, catalysts are typically sprayed onto both sides of the PEM to form the catalyst coating, with iridium oxide employed as the anode catalyst and platinum-carbon used as the cathode catalyst.

The porous transport layer (PTL) and bipolar plates also play pivotal roles within the PEM water electrolysis (PEMWE) system. The PTL primarily supplies input channels for reactants and output channels for products while functioning as an electronic conductor to facilitate the connection between the MEA and the external circuit. Bipolar plates are mainly designed to conduct current and feature specific flow channels to expedite fluid transport. Moreover, they serve to separate battery cells, preventing the mixing of hydrogen and oxygen, and provide structural support for the gas diffusion layer (GDL) and MEA, thereby ensuring the overall stability of the system.

## 3 Research and development of electrolyte membranes

In recent years, remarkable achievements have been made in the field of proton exchange membrane. As a key component of PEMWE technology, the proton exchange membrane needs to have high proton conductivity, low gas permeability, good chemical stability, and mechanical strength [11]. In addition, ultra-thin and high-temperature proton exchange membranes have become important development trends for the future. These research directions open up new ideas for commercial application of proton exchange membrane technology and provide more solutions. The selection of proton exchange membrane (PEM) is usually based on the following criteria: high proton conductivity, low gas permeability, good mechanical properties, high chemical stability, and appropriate thickness uniformity [12]. At present, the commonly used proton exchange membrane (PEM) materials mainly include perfluorosulfonic acid membrane, represented by Nafion membrane of DuPont Company, which has excellent chemical stability, proton conductivity and mechanical properties; Some fluorinated sulfonic acid membranes, such as BAM3G membrane, have good chemical stability and mechanical strength; non-fluorinated sulfonic acid membranes, sulfonated polyether ether ketone (SPEEK) is the representative of this type of membrane, which is low in cost and easy to process; composite membranes, such as polytetrafluoroethylene (ePTFE) reinforced composite membranes developed by Gore Company, have higher mechanical strength and proton conductivity and polybenzimidazole (PBI)/H PO membranes, which are suitable for high temperature proton exchange membrane fuel cells.

## 4 Design and optimization of gas diffusion layer

The design of the gas diffusion layer (GDL) is critical to the performance of the PEMWE system. The optimization direction covers many aspects such as pore structure design, material selection, microporous layer design, and wettability adjustment. It has been found that lower fiber concentration and compression ratio are conducive to achieving maximum diffusion, while higher fiber concentration and compression ratio are conducive to improving conductivity [13]. In addition, reasonable adjustment of pore size distribution and channel geometry can significantly improve oxygen transmission efficiency and enhance water management capabilities. The application of new metal foam materials and the development of 3D printing technology provide innovative ideas for high performance design of GDL. Gas Diffusion Layer (GDL) performs a variety of important functions in PEMWE systems, including supporting catalyst layers and transporting reactant gases and products (such as hydrogen, oxygen/air, water, etc.) and conducting current. To ensure that the gas diffusion layer can function effectively, it should meet the following requirements: the material selected must be suitable for supporting the catalytic layer, and the contact between the diffusion layer and the catalytic layer The resistance should be small; the diffusion layer should have a suitable void fraction and a reasonable pore distribution to facilitate material transport; the diffusion layer must be a good electrical conductor and maintain good resistance parallelism in both the horizontal and vertical directions; The diffusion layer should have good heat transmission and distribution ability to ensure the uniformity of the power generation process and help to prolong the service life of the membrane electrode; the diffusion layer should have strong corrosion resistance to ensure the durability and stable performance output of the system. The commonly used gas diffusion layer materials include carbon fiber paper, carbon fiber woven cloth, carbon fiber nonwoven fabric, and carbon black paper [14]. In terms of preparation technology, carbon fiber paper can be prepared by dry forming or wet forming. The gas diffusion layer has many advantages, such as high mechanical strength, excellent electrical conductivity, good gas diffusion ability, and chemical stability. However, it also has some disadvantages, such as high production costs and during long-term operation, the surface catalytic layer may be blocked, thus affecting the system performance [15].

## 5 The technological development and challenges of bipolar plates

Bipolar plates (BPPs) play an indispensable role in proton exchange membrane water electrolyzers (PEMWE). It is not only able to separate the cell, effectively prevent hydrogen and oxygen mixing, but also responsible for the uniform distribution of reaction gases, as well as the conduction of current and heat. In addition, the bipolar plate provides the necessary structural support for the gas diffusion layer (GDL) and the membrane electrode assembly (MEA), which plays a key role in maintaining the stability of the system. Therefore, the conductivity, corrosion resistance and mechanical strength of bipolar plates are directly related to the efficiency and long-term operation performance of PEMWE system [16,17].

The choice of bipolar plate material has a direct impact on the performance and cost of the PEMWE system. Commonly used bipolar plate materials include titanium (Ti), stainless steel (SS), and nickel alloys etc. These materials have good electrical and thermal conductivity. However, in the high-potential and strong-acid environment of the PEMWE system, metal materials are prone to corrosion [17,18]. Titanium is widely used because of its excellent corrosion resistance, however, its high cost and the existence of the hydrogen embrittlement problem limit its large-scale use [18]. In contrast, stainless steel is cheaper and easier to process, but under high potential conditions, chromium and iron in stainless steel will dissolve, which may poison the membrane electrode assembly (MEA), which in turn affects system performance.

To improve the corrosion resistance and reduce the cost of the double plate, the researchers used the coating technology, such as in the stainless steel surface coated with titanium, which provides resistance to corrosion of metal. The platinum coating significantly improves the corrosion resistance of the material and maintains good electrical properties in the PEMWE environment. However, it should be noted that these coatings may degrade under high potential and high temperature environments, resulting in peeling or cracking of the coating, thus affecting its protective performance [9]. Therefore, optimizing the stability and long-term performance of coatings has become the focus of current research.

As a bipolar plate material, stainless steel has the advantages of high mechanical strength, good conductivity, and low cost. However, its corrosion in high-potential and strong-acid environments greatly limits its application in PEMWE systems [18]. Corrosion resistance and long-term stability of stainless steel can be significantly improved by coating with titanium, platinum, and other corrosion-resistant coatings [17]. However, during long-term use, the coating may be damaged, especially in the case of current fluctuations at high potentials, and the coating is more prone to degradation [15]. Therefore, the development of more corrosion-resistant and stable coating materials to improve the durability of the coating is the key issue to be solved in the current research of bipolar plate technology.

# 6 Current situation and limitations of PEMWE technology

## 6.1 Technical bottlenecks and challenges

Although proton exchange membrane water electrolyzers (PEMWE) technology has the advantages of high efficiency and fast dynamic response, there are still some technical difficulties to be broken through in practical application. Among them, the problems of high potential corrosion and acid environment erosion faced by bipolar plate materials during operation seriously affect the service life and reliability of the system. Although the corrosion rate of the bipolar plate can be temporarily alleviated by surface coating treatment, the structural stability and durability of the existing coating is still facing a severe test - under long-term complex working conditions, the protection performance of the coating will gradually deteriorate, and the protection failure will be caused by the weakening of the interface binding force, which will lead to the continuous decline of the system performance. These core problems have become the main obstacles restricting the large-scale application of PEMWE technology.

## 6.2 Future development direction and potential improvement measures

Future research should focus on three core directions: the development of bipolar plate substrate with high potential corrosion resistance at the material system level; In the field of surface engineering, the interface bonding strength and environmental aging resistance of the coating are improved. Through large-scale preparation and structural design optimization, cost reduction and efficiency increase are realized in the manufacturing process. At the same time, the comprehensive stability of bipolar plate components under strong acid and high potential conditions is continuously improved through multi-dimensional collaborative innovation, to build a more competitive market industrialization foundation for PEMWE technology. On this basis, promoting the iterative upgrading of material-process-equipment will accelerate the leap of this technology to the stage of large-scale commercial application.

## 7 Conclusion

At present, PEMWE technology has matured. In summary, PEM has been commercialized with high proton conductivity. GDL, thanks to 3D printing, develops rapidly but faces cost and blocking issues. Coating technology can deal with the problems of bipolar plate material, but it needs a more stable coating material. Above all, the deficiency of coating material is the most restrictive to the development of PEMWE. This paper believes that more efforts should be taken to innovate the coating technology. By enhancing the durability of the coating, bipolar plate challenges can be resolved and the electrolyzer life can be extended, which can accelerate PEMWE commercialization, boost its influence in the field of hydrgen-production and become a key environmental solution.

## Authors Contribution

All the authors contributed equally, and their names were listed in alphabetical order.

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