Optimizing Green Hydrogen Production: A Computational Simulation of Proton Exchange Membrane Electrolysis

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ABSTRACT

The present work aims to perform a computational simulation of a Proton Exchange Membrane (PEM) reactor in the water electrolysis process for green hydrogen production using Ansys Fluent software. The geometry of the electrolyzer was designed using Solid Edge software, followed by a mesh quality study. Subsequently, the current density was analyzed by varying voltage values between 1.0V and 14.0V, and a polarization curve of electric voltage as a function of current density was generated. This work has the potential to contribute in the development of more efficient and commercially viable PEM electrolyzers.

Keywords: Electrolysis; Hydrogen Production; Simulation; Proton Exchange Membrane.

INTRODUCTION

Proton exchange membrane (PEM) water electrolysis technology stands out due to its simple design and capability to operate at high current densities under low temperatures, producing high-purity hydrogen (Bessarabov *et al.*, 2015). This work aims to simulate PEM electrolysis using ANSYS-Fluent software to analyze the current density and generate a polarization curve, plotting electric voltage relative to current density. The key component of PEM electrolyzers is the proton exchange membrane (**Fig. 1**), also known as a solid polymer electrolyte. This membrane separates the cathode from the anode, allowing the electrolyzer to operate at low temperatures, typically between 80 and 150°C, and at pressures up to 400 bar (Salehmin *et al.*, 2022). The electrodes, which can be made of various materials, must exhibit high chemical stability and excellent electrical conductivity, as the electric current is indirectly responsible for breaking down water molecules to produce hydrogen and oxygen gases.

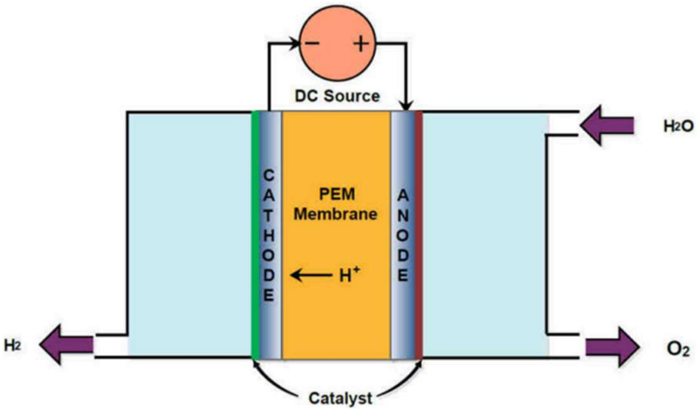

Figure 1: PEM Electrolysis Diagram.

When designing a PEM electrolyzer, three primary factors must be considered: performance, durability, and cost. Upon applying current to the cell, water is split into hydrogen and oxygen, with hydrogen protons passing through the membrane to form hydrogen gas on the cathode side. A critical challenge in making this process economically viable lies in reducing infrastructure costs and developing technologies that enhance efficiency, such as lowering cell voltage, improving energy density, and controlling pressure and temperature. Further advances in membrane and channel materials will also help optimize the system.

MATERIALS AND METHODS

A geometric model of the electrolyzer was constructed in Solid Edge software, adhering to the design specifications by Juan (2023). In the software, current collectors are modeled as solid bodies, while other components are treated as fluid volumes. Each part of the cell is labeled to ensure the software correctly identifies the components' positions relative to the electrodes.

After defining the geometry, it was exported to ANSYS Workbench to generate the reactor mesh. The final mesh contained 165,600 elements (**Fig. 2**), with distortion and orthogonality coefficients of 0.08 and 0.97, respectively, indicating a high-quality mesh.

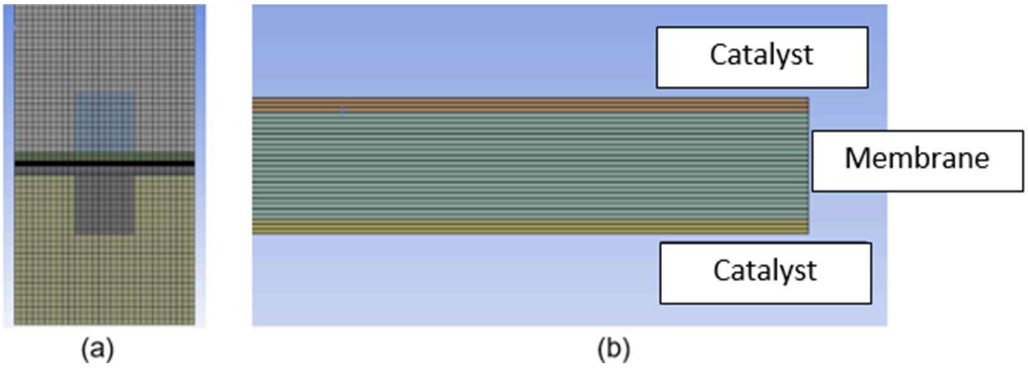

Figure 2: Mesh generated in the Z-Y plane (5a); Mesh on the catalysts and membrane, X-Y plane (5b).

In electrolysis systems, two potential equations are solved to describe the system (Ansys, 2023). The first equation, related to electron transport in the solid zones of the different layers, defines the potential as φ_{sol}.

$$\nabla.(\sigma_{sol}\nabla\varphi_{sol}) + R_{sol} = 0 \qquad Eq.\ (1)$$

The second equation describes ion transport in the electrolytic membrane, where the potential is defined as φ_{mem}:

$$\nabla.(\sigma_{mem}\nabla\varphi_{mem}) + R_{mem} = 0 \qquad Eq.\ (2)$$

where σ refers to electrical conductivity in the solid zones and ionic conductivity in the fluid zones, while R represents the volumetric transfer current. The subscripts "sol" and "mem" correspond to the solid and membrane phases, respectively. The potential difference between these phases indicates the surface potential, driving the electrochemical reactions.

σ = electrical conductivity (1/ohm.m)

R = volumetric transfer current (A/m^3)

Boundary conditions for φ_{sol} and φ_{mem} are defined over the entire computational domain. No ionic current flows beyond the electrolyzer's outer boundaries, meaning that ions produced by the reactions remain within the system. However, electrons can pass through the boundaries of the current collectors (anode and cathode tabs), which are in contact with the external electrical circuit. Here, either a fixed potential value or a potential flux condition is applied.

After defining the boundary conditions, we return to the two potential equations. The source terms R_{sol} and R_{mem} represent the transfer currents at the anode and cathode, respectively, expressed as:

$$R_{an} = \left(\delta_{an}\, j_{an}^{ref}\right)\left(\frac{|A|}{|A|_{ref}}\right)^{y_{an}}\left(e^{\frac{+\alpha_{an}F\omega_{an}}{RT}} - e^{\frac{-\alpha_{an}F\omega_{an}}{RT}}\right) \qquad Eq.\ (3)$$

$$R_{cat} = \left(\delta_{cat}\, j_{cat}^{ref}\right)\left(\frac{|C|}{|C|_{ref}}\right)^{y_{cat}}\left(-e^{\frac{+\alpha_{cat}F\omega_{cat}}{RT}} + e^{\frac{-\alpha_{cat}F\omega_{cat}}{RT}}\right) \qquad Eq.\ (4)$$

Where, j^{ref} represents the reference exchange current density per active surface area (A/m^2); δ is the specific active surface area (1/m); α is the transfer coefficient (dimensionless); F is the Faraday constant (96,485 C/mol); $|A|$ *and* $|C|$ are local concentrations of the species on the anode and cathode sides, respectively (kmol/m^3); $|A|_{ref}$ *and* $|B|_{ref}$ are the concentration of the species in the reference state (kmol/m^3).

The local surface overpotential ω is the difference between the solid and membrane potentials:

$$\omega_{an\ or\ cat} = \varphi_{sol} - \varphi_{mem} \qquad Eq.\ (5)$$

The electrical potential inside the electrolyzer increases, and this gain is adjusted by subtracting the open-circuit voltage V_{oc}:

$$\omega_{an\ or\ cat} = \varphi_{sol} - \varphi_{mem} - V_{oc} \qquad Eq.\ (6)$$

RESULTS AND DISCUSSION

To acquire accurate data on heat and mass transfer, as well as electrolyzer performance, the project employed computational simulations combining computational fluid dynamics (CFD) with electrochemical modeling of the electrolysis process using ANSYS-Fluent software (**Fig. 3**).

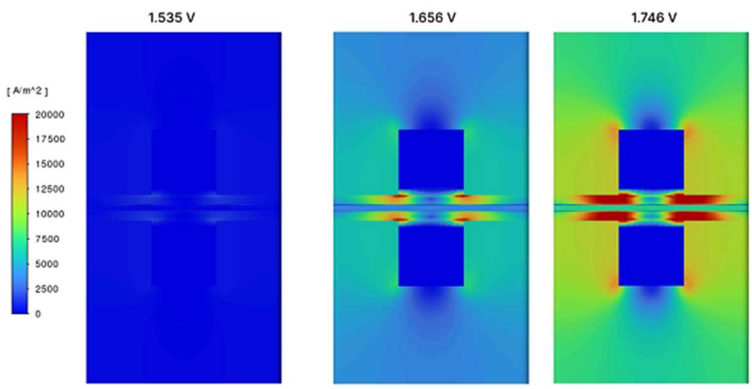

Figure 3: Example of computational simulation: current density contours in a PEM electrolysis cell for different voltages (V).

Typically, electrolysis produces hydrogen and oxygen gases, meaning that the system functions as a gas-liquid multiphase fluid system. The analysis includes the simulation of polarization curves, which represent the relationship between current density and electric voltage (**Fig. 4**).

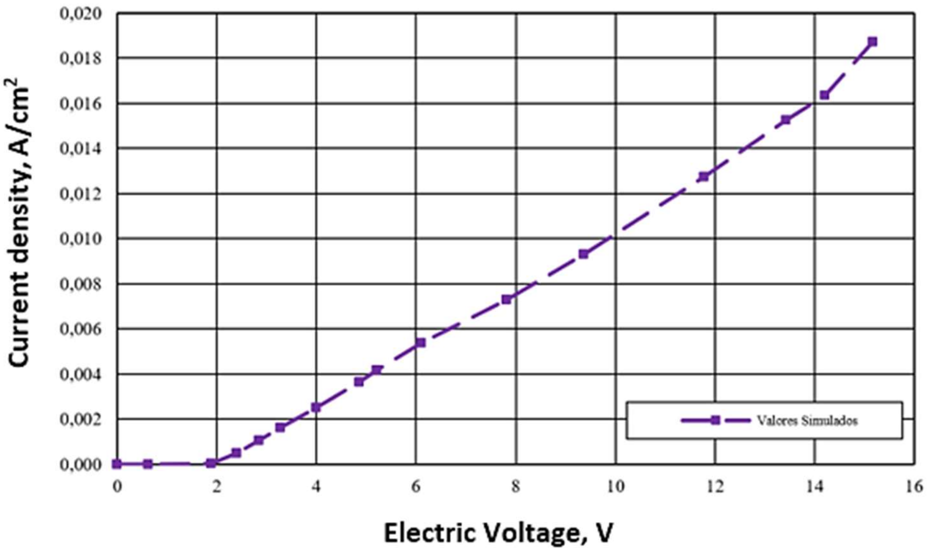

Figure 4: Electrolyzer polarization curve.

CONCLUSION

This work has the potential to contribute significantly to the advancement of green hydrogen technology, specifically in the development of more efficient and commercially viable PEM electrolyzers. The computer simulations will provide an in-depth understanding of the membrane characteristics, facilitating its large-scale production and attracting investments.

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