

Modeling and Simulation of Proton Exchange Membrane Water Electrolyzer and Application of Model Order Reduction on Its Power Rails

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Introduction

The Proton Exchange Membrane Water Electrolyzer (PEMWE) is steadily gaining recognition as a paramount technology for pollution-free hydrogen production. A detailed understanding and representation of its internal physical processes are crucial for optimizing its hydrogen production efficiency. In this research, we present a comprehensive three-dimensional single-phase model of the PEMWE based on computational fluid dynamics (CFD) utilizing the finite volume method (FVM).

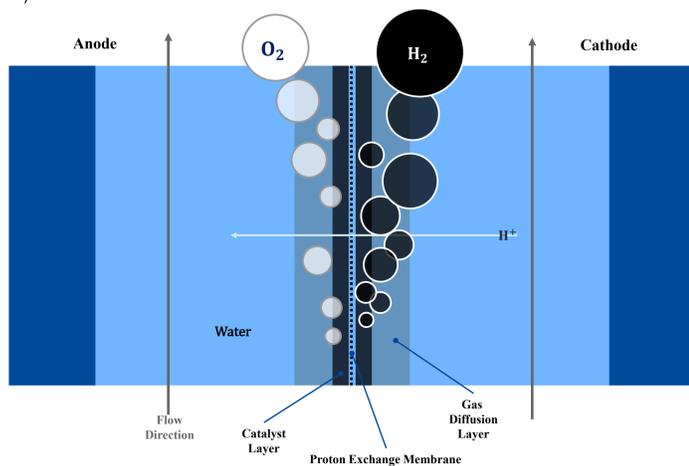
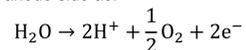


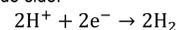
Figure 1: Schematic of PEMWE.

The PEMWE has symmetric structure, which comprises bipolar plate, channel, gas diffusion layer, and catalyst layer in both sides, as shown in Figure 1.

The oxygen is generated on the anode side as:



and hydrogen is generated on cathode side:



Model Description

The single-phase PEMWE is modeled in ANSYS Fluent. Its computational domain is depicted in Figure 2. A positive potential is applied to the outer surface of the anode bipolar plate, while the potential of the cathode bipolar plate is fixed to 0.

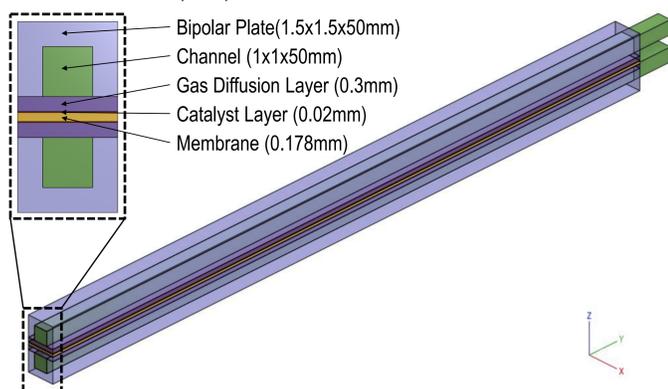


Figure 2: The structural design and computational domain of the PEMWE.

Based on the modified Butler-Volmer equation, the expression of volumetric transfer current j can be calculated as follows [1]:

$$j_a = \xi_a i_a \frac{C_{\text{H}_2\text{O}}}{C_{\text{H}_2\text{O},ref}} \left[\exp\left(\frac{\alpha_a F}{RT} \eta_a\right) - \exp\left(\frac{(1-\alpha_a)F}{RT} \eta_a\right) \right]$$

$$j_c = \xi_c i_c \left[\exp\left(\frac{\alpha_c F}{RT} \eta_c\right) - \exp\left(\frac{(1-\alpha_c)F}{RT} \eta_c\right) \right]$$

where a and c in subscripts stand for anode and cathode, respectively. ξ is the specific active surface area, i is the exchange current density, $C_{\text{H}_2\text{O}}$ and $C_{\text{H}_2\text{O},ref}$ are the local water molar concentration and reference water molar concentration, α is the transfer coefficient, F is the Faraday constant, R is the universal gas constant, T is the temperature.

η is the activation overpotential given by

$$\eta_a = \phi_s - \phi_m - E_{eq}$$

$$\eta_c = \phi_s - \phi_m$$

where ϕ_s is solid phase potential, ϕ_m is the membrane phase potential, and E_{eq} is the equilibrium voltage.

The anodic and cathodic exchange current densities are written as

$$i_a = i_a^{ref} \left[\frac{-E_{act,a}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]$$

$$i_c = i_c^{ref} \left[\frac{-E_{act,c}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]$$

where i^{ref} is the reference current density, E_{act} is activation energy, and T_{ref} is the reference temperature.

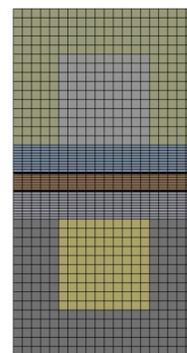


Figure 4: The mesh of the computational domain.

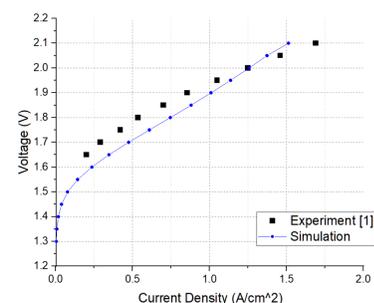


Figure 5: Comparison of the polarization curve against experimental data [1].

The developed model exhibits commendable agreement with experimental findings as shown in Figure 5, underlining its accuracy and potential utility in real-world applications.

Power Rails and the Application of Model Order Reduction

A pivotal aspect of a holistic system-level simulation of a complete hydrogen generation plant is the power rails, which are specially designed for the electrolyzer's power transmission. We have modeled these power rails with meticulous attention to both electromagnetic and thermal effects. Through solving the electromagnetic field of the power rails, we obtain the ohmic loss distributions, which will be the inputs as heat generation rate of the thermal model. The temperature distribution will be computed in the thermal model and provides feedback to the EM model accordingly. Since the electrical resistance of the power rails varies with temperature and causes to different ohmic losses. The implementation of two-way coupling enables us to accurately determine the temperature-dependent power loss.

A major challenge with intricate models is the computational demand. Both models will be computed multiple times and exchange data in an iterative process until the results meet the convergence criteria. To overcome this, we have applied projected-based model order reduction (MOR) to the power rails, resulting in the streamlined, reduced-order models (ROM) extracted from the full Finite Element Method (FEM) models. This approach has significantly cut down on computation time, enabling faster, and potentially real-time, system-level simulations.

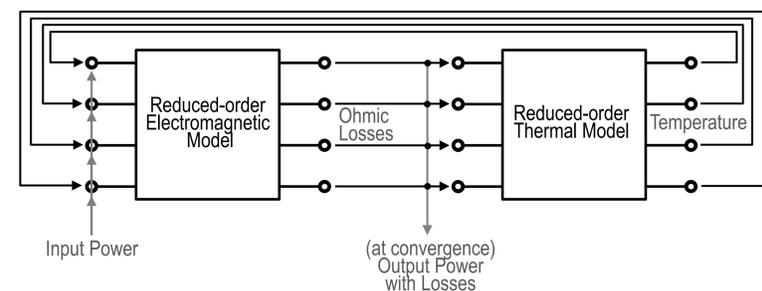


Figure 6: Flowchart of two-way coupling of the electromagnetic ROM and thermal ROM.

References

- [1] Zhou, H., et al. "3D two-phase and non-isothermal modeling for PEM water electrolyzer: Heat and mass transfer characteristic investigation." Int J Energy Res. 46 (2022): 17126–17143.