

Multiscale and Multiphysics 1D Modeling of a PEM Water Electrolyser

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Polymer Electrolyte Membrane Water Electrolysers (PEMWEs) are particularly promising for coupling with intermittent renewable energy. However, their widespread adoption is hindered by durability challenges, as dynamic operating conditions can accelerate degradation mechanisms within the Membrane Electrode Assembly (MEA) [1]. Understanding the interplay between local thermodynamic conditions and material degradation is crucial for developing mitigation strategies.

We present the development of a one-dimensional (1D), through-plane, multiphysics model of a PEMWE, focusing on the coupling between electrochemical phenomena and multiphase fluid dynamics [2]. The model resolves the physical phenomena across the main components of the electrolyser: the Porous Transport Layers (PTLs), Catalyst Layers (CLs), and the membrane.

The model integrates three strongly coupled physical domains. The distribution of electric and ionic potentials is described by Poisson's equation. Electron transport is modeled in the solid phases (PTLs and CLs), while proton transport is considered in the ionomer phase (CLs and membrane). The transport of reactants (liquid water) and products (gaseous H₂ and O₂) through the porous layers is described by a compositional multiphase flow model. Mass conservation equations are formulated for each phase, while the velocity fields are determined by Darcy's law, accounting for capillary pressure effects at the liquid-gas interface. The reaction terms for the charge and mass balance equations are governed by Butler-Volmer kinetics.

The model is implemented in Python using the FEniCSx finite element computing platform, with the MultiPhenicsx library employed to manage the coupled system. The steady-state electrochemical part of the model has been successfully solved, as presented in [3].

The current focus is on solving the transient, non-linear system of PDEs for the fluid dynamics. This presents significant numerical challenges due to the stiff nature and tight coupling of the equations for saturation, pressure, and mass fraction. Various solver strategies are being investigated to achieve robust convergence for the fully coupled multiphysics problem.

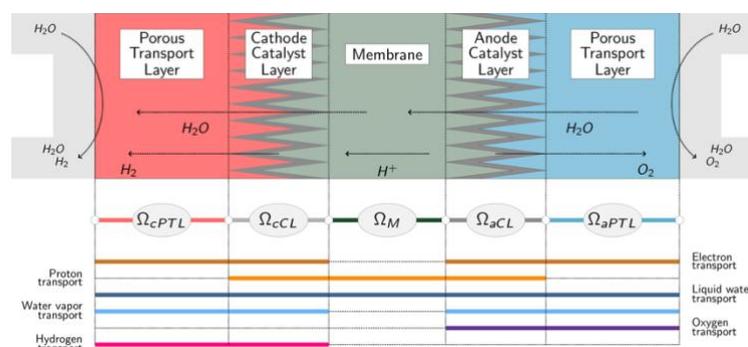


Figure 1 - Visual representation of the PEMWE and its components; distribution of the different phenomena in the various subdomains.

[1] Q. Feng, X.-Z. Yuan, G. Liu, B. Wei, Z. Zhang, H. Li, and H. Wang, «A Review of Proton Exchange Membrane Water Electrolysis on Degradation Mechanisms and Mitigation Strategies», Journal of Power Sources, vol. 366, pp. 33-55, Oct. 2017.

[2] N. Lin, S. Feng, and J. Wang, «Multiphysics Modeling of Proton Exchange Membrane Water Electrolysis: From Steady to Dynamic Behavior», AIChE Journal, vol. 68, no. 8, p. e17742, Aug. 2022.

[3] S. Pierobon, R. Tittarelli, Z. Li, «Multiscale and Multiphysics 1D Modeling of Polymer Electrolyte Membrane Water Electrolysers.» Symposium de Génie Electrique (SGE 2025), Toulouse, France.