

New frontiers in State-of-the-Art PEMFC Modeling: Insights from a Comprehensive Transient Experimental Validation

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Proton exchange membrane fuel cells (PEMFCs) have gained significant traction in recent years with industrialization efforts ramping up world-wide. However, obtaining optimal performance from these cells hinges on a thorough understanding of their complex electrochemical behavior across a wide range of conditions. A shortcoming of current PEMFC modeling is the lack of comprehensive validation. Many studies rely on few single polarization curves and neglect the complexities of transient effects. However, only through the simulation of dedicated transient experiments, subtleties of water management and the associated timescales particularly relevant for stack and system simulations can be revealed. As a result, current models have limited predictive qualities, with their validity being confined to specific conditions or different parameter sets being required for each combination of temperature and relative humidity. Our study aims to address this gap by rigorously validating a state-of-the-art 2D, transient, non-isothermal PEMFC model (fig. 1), based on works by several research groups [1-4]. Utilizing a unified set of parameters, we have conducted a comprehensive validation across a wide spectrum of temperatures and relative humidities through polarization curves, electrochemical impedance spectroscopy (fig. 2), limiting current measurements, and recently developed transient experiments designed to probe changes in water saturation.

Our analysis exposes the strengths and limitations of the model. It reveals areas with the greatest necessity for additional research and clearly identifies the most critical challenges where further model advancement is required, with a focus on water management, ageing mechanisms and general transient effects. These aspects are of vital importance for the development and application of comprehensive modeling tools that succeed in bridging scales from component to single cell to stack levels.

[1] Pant, L. M., Gerhardt, M. R., Macauley, N., Mukundan, R., Borup, R. L., & Weber, A. Z. (2019). Along-the-channel modeling and analysis of PEFCs at low stoichiometry: Development of a 1+ 2D model. *Electrochimica Acta*, 326, 134963.

[2] Vetter, R., & Schumacher, J. O. (2019). Experimental parameter uncertainty in PEMFC modeling. Part I: Scatter in material parameterization. *Journal of Power Sources*, 438, 227018.

[3] Eikerling, M. H., & Berg, P. (2011). Poro-electroelastic theory of water sorption and swelling in polymer electrolyte membranes. *Soft matter*, 7(13), 5976-5990.

[4] Goshtasbi, A., García-Salaberri, P., Chen, J., Talukdar, K., Sanchez, D. G., & Ersal, T. (2019). Through-the-membrane transient phenomena in PEM fuel cells: A modeling study. *Journal of The Electrochemical Society*, 166(7), F3154.

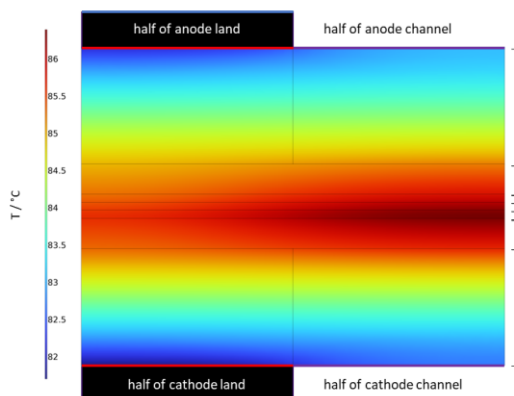


Figure 1: Temperature distribution across model geometry.

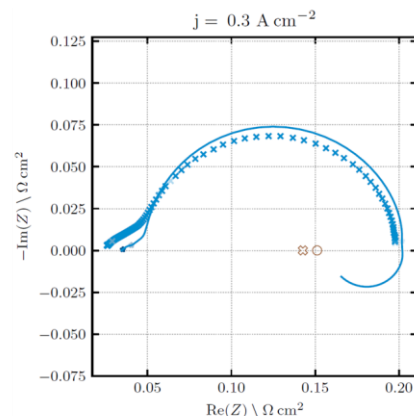


Figure 2: Model validation through EIS.