CFD modeling of a PEM water electrolyzer: relationship between flow regime and performance

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The relationships between operating conditions, two-phase flow regime in the anode channel, and performance of a polymer electrolyte membrane water electrolyzer (PEMWE) is not well understood. These relationships are important for optimizing cell operation in view of power consumption and stability. To address this issue, a model for the interplay of the relative velocity between the two phases and the bubble diameter in the anode channel is developed. It accounts for the effect of current density on the bubble diameter using fitting to experimental data as input [1]. This model is coupled with the electrochemical kinetics in catalyst layers to perform 3-D computational fluid dynamics (CFD) simulations of a PEMWE (Fig. 1) in the open-source platform OpenFOAM. The operating point is defined by the average area current density *i*, and the water stoichiometry λ. The two-phase flow regime is quantified by the normalized flow regime number, *frn**, and the cell performance is characterized by the cell voltage, *U*. The model is compared to the experimental data of two-phase flow reported in Ref. [2]. Results show that the *frn** provides a criterion to distinguish the three main flow regimes (bubbly, plug, and slug). Simulation results help furnish relationships between operating point, flow regime and cell performance. The best cell performance (lowest cell voltage) is found to occur at the highest water stoichiometry, $\lambda = 1000$, in simulations, where the bubbly flow regime prevails for current densities from 0.1 A/cm^2 to 2.0 A/cm^2. Slug flow with the highest value of *frn** appears at 0.8 A/cm^2 with the lowest water stoichiometry 100 (Fig. 2) due to the high oxygen volume fraction. Among other findings, it demonstrates that the water stoichiometry should be increased to decrease cell voltage and oxygen bubble sizes in the anode channel. This work provides important basic trends and limiting values for cell operation.

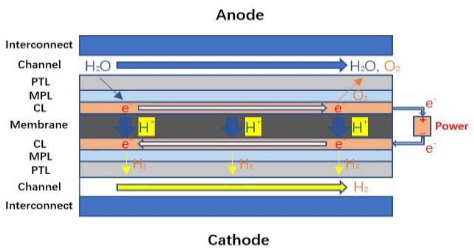

Figure 1: Principle and physical structure of the PEM electrolyzer model (dead end of cathode inlet)

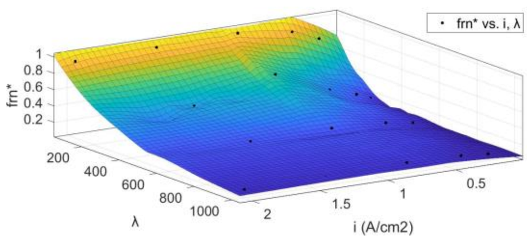

Figure 2: Relationship between operating point and normalized flow regime number

1. Zhang, T., Cao, Y. et al. *Journal of Power Sources* **2022**, 542, 231742. DOI: 10.1016/j.jpowsour.2022.231742
2. Panchenko, O., Giesenberg, L. et al. *Energies* **2019**, 12(3), 350. DOI: 10.3390/en12030350