PEM electrolysis model with experimental validation

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To meet the ever growing demand for polymer electrolyte membrane (PEM) electrolyzers to operate at higher current densities, higher pressures and higher temperatures [1], a zero dimensional simulation was developed that can be used to optimize operating conditions and cell geometries. The model presented in this research was focused on capturing the performance of an electrolyzer operating at higher current densities ranging from 2-6 A/cm^2. This entails focusing more on the mass transport and ohmic losses (both proton transport and electron transport related) that dominate under these conditions.

Modeling in electrolysis originally began by simply modifying a PEM fuel cell model and applying the electrolysis boundary conditions [2]. This can in some cases be problematic as many of the operating regimes found in PEM electrolysis are quite different than those found in a PEM fuel cell [3]. For instance, because the reaction is reversed water is supplied to the catalyst while oxygen and hydrogen must be removed, while the opposite is true for PEM fuel cells. Removing a gas from the catalyst layer is much easier due to their lower densities (less inertia) and higher diffusivities, thus reducing the onset of mass transport losses. This is what allows the PEM electrolyzer to operate at such high current densities when compared to PEM fuel cells, however, it prompts changes in how the mass transport losses are to be accounted for.

Due to the vast similarities between the PEM electrolyzer and the PEM fuel cell, a large database of simulations, each with their own specialty, are available in the literature [3]. By combining the strengths of the individual models from both, fuel cell and electrolysis to each sub-model used in this analysis, a design tool was developed to optimize operational and geometrical parameters of a PEM electrolyzer. Models with a strong focus on ohmic losses similar to the electrical resistance model developed by Marangio *et al.* [4] and models specifically developed for the prediction of membrane proton conductivity like that of Choi *et al.* [5] were combined to improve the prediction of the ohmic losses. These are particularly important when operating a cell at high current densities due to the linear dependence with current density ohmic losses have on the cell operation. Figure 1 illustrates simulated and experimental performance curves for a single cell PEM electrolyzer operating at 50°C and 80°C.

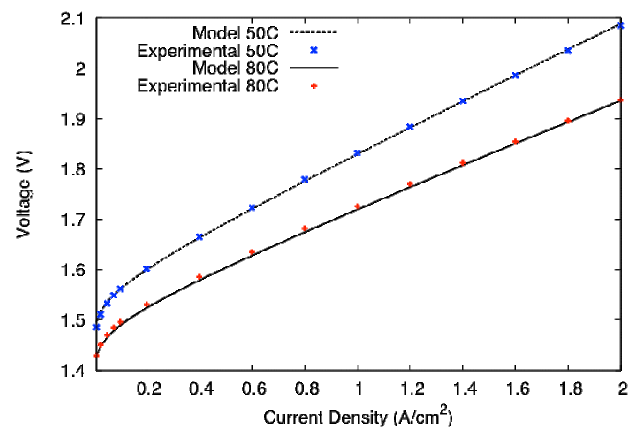

Figure 1: Single cell PEM electrolyzer experimental results and model validation of a 25 cm^2 active area cell.

With the model validated under various operating conditions, a separator plate/flow field design optimization was performed. This was conducted with the goal of maximizing the contact area between the surface of the porous transport layer and the separator plate.

In conclusion, a new, robust and computationally efficient design tool is introduced capable of optimizing many geometrical and operational parameters of a PEM electrolysis cell. This model was validated and used to perform an optimization study on the design of the separator plate.

References

[1] J. Mergel, M. Carmo and D. Fritz. *Transition to Renewable Energy:Status on Technologies for Hydrogen Production by Water Electrolysis*, D. Stolten, V. Scherer, Editors, p. 423-450, Wiley-VCH, Weinheim (2013)

[2] K. Onda, T. Murakami, T. Hikosaka, M. Kobayashi, R. Notu and K. Ito. *Journal of the Electrochemical Society*, **149**, (8), A1069-A1078 (2002)

[3] M. Carmo, D. Fritz, J. Mergel and D. Stolten, *International Journal of Hydrogen Energy*, **38**, 4901-4934 (2013)

[4] F. Marangio, M. Santarelli and M. Cali, *International Journal of Hydrogen Energy*, **34**, 1143-1158 (2009)

[5] P. Choi, N. Jalani and D. Ravindra, *Journal of the Electrochemical Society*, **152**, (3), E123-E130 (2005)