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## Heterogeneous Wettability in Porous Catalyst Layers of PEM Fuel Cells: Modeling-based Analysis and Design

*Tuesday, 1 June 2021 10:00 (1 hour)*

Polymer electrolyte membrane (PEM) fuel cells are expected to play an integral role as low-emission energy converters in a future energy economy. Although technological maturity of these cells has been demonstrated, the challenge remains to achieve high power performance at drastically reduced platinum loading. So far, the attempts to reduce the platinum loading have been thwarted by severe voltage losses. A possible origin of these losses is the water flooding of porous gas-transport media. The optimal water balance is of particular importance for the operation of the cathode catalyst layer (CCL), wherein liquid water is needed for efficient proton transport and high activity of the oxygen reduction reaction [1], whereas excessive water accumulation in pores (i.e., flooding) would block the porous pathways needed for the gaseous supply of oxygen. An optimal design of porous electrode media PEM fuel cells should thus account for heterogeneous wettability effects in them.

Conventional CCLs possess an agglomerate structure with a bimodal porous network morphology [2]. Primary pores (1-10 nm diameter) exist in the carbon support, which has platinum particles (1-5 nm diameter) attached to its surface. Secondary pores (10 –50 nm diameter) form the space between Pt-loaded carbon. An ionomer-subphase is dispersed in this structure, forming a thin, skin-like layer that partially covers the surface of Pt/C particles or their agglomerates.

The CCL exhibits a highly heterogeneous wetting behavior. Various models [3, 4] account for the impact of the mixed wettability, parametrizing contact angles and fractions of hydrophilic/hydrophobic parts independently to match experimental data. We propose a novel approach that harnesses the correlations between the wetting behavior and the structure and composition of the layer. The main distinction is made between ionomer-penetrated and ionomer-free pores. The impact of the Pt particle density on the support is also explicitly considered. Moreover, a peculiar ionomer inversion effect that had been seen in previous experimental results plays a crucial role: where ionomer covers the Pt/C surface, previously hydrophilic surfaces turn hydrophobic [5]. Consequently, we developed a set of descriptors, including a statistical density function for wetting properties. Our analysis of the relations between structure, composition, wettability and performance supports the following hypothesis: lowering the Pt loading via reducing the Pt:C ratio evokes hydrophilic wetting behavior in secondary pores, leaving the CCL highly susceptible for flooding. Based on this finding, we derive design strategies to match low-Pt-loading with flooding-resistant wetting behavior. The results of this work are embedded in larger framework of a comprehensive, structure-based model to link CCL recipe and material choices with performance.

### Time Block Preference

Time Block A (09:00-12:00 CET)

### References

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- [5] Y. M. Volfkovich, V. E. Sosenkin, and V. S. Bagotsky, "Structural and wetting properties of fuel cell components," *Journal of Power Sources*, vol. 195, no. 17, pp. 5429–5441, Sep. 2010, <https://doi.org/10.1016/j.jpowsour.2010.03.002>

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