Coupling of deterministic contact mechanics model and two-phase model to study the effect of catalyst layer|microporous layer interface on polymer electrolyte fuel cell performance

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Water accumulation and Ohmic losses at catalyst layer (CL)|micro-porous layer (MPL) interface inside polymer electrolyte fuel cell (PEFC) can potentially have a critical role in the electrode's performance (1, 2). Interfacial gaps can act as water-pooling voids hindering reactant transport to the CL. Moreover, imperfect interfacial contact can create high-resistance electron pathways between the CL and MPL.

We present an elastic deterministic contact mechanics model for studying interfacial morphology at CL|MPL interface (3). The model uses the surface height data of the CL and MPL samples obtained with optical microscopy technique as an input to generate three-dimensional interfacial gap profiles under different levels of compression (3). We pair two different sets of CLs and MPLs: 1) SGL 10BC Sigracet GDL, abbreviated as SGL and an Ion Power MEA, abbreviated as IP, 2) MRC U105 carbon paper with an MPL and a Gore Primea MEA. The generated water-retention curves and average spatial distributions are input into a macroscopic two-phase, two-dimensional PEFC model to investigate the influence of the CL|MPL interface on the overall PEFC performance. The CL|MPL interface is incorporated as a finite-thickness, two-dimensional domain, where the capillary pressure - saturation relation is described with van Genuchten curves that are generated from the deterministic model.

Figure 1 shows through-plane saturation profiles for the IP|SGL interface at RH = 100% for the compressed interface (p = 1 MPa). The PEFC's domains are marked and the inset shows a zoom-in view of saturation at the CL|MPL interface. We plot saturation profiles for the PEFC's potentials of 0.85 and 0.4 V. The solid lines show saturation profile if the CL|MPL interface had MPL properties, while the dashed lines show the saturation profile when the CL|MPL interface is included in the model. We observe high saturation values at the CL|MPL interface due to large cracks present on the surface of the SGL sample that act as water-pooling voids.

Based on the interfacial saturation values generated with the two-phase PEFC's model we were able to generate local three-dimensional interfacial water distributions with deterministic contact mechanics model. We used three-dimensional morphological opening procedure with spherical kernel to evaluate the interfacial void space as a function of critical radius of curvature. Figures 2a and 2b show three-dimensional interfacial water distributions for the IP|SGL interface at the operating conditions corresponding to Figure 1. At high current densities there is more water generated and smaller interfacial voids are filled with water as shown by Figure 2b. For low current densities mostly large voids that correspond to deep cracks at the SGL surface are filled with water.

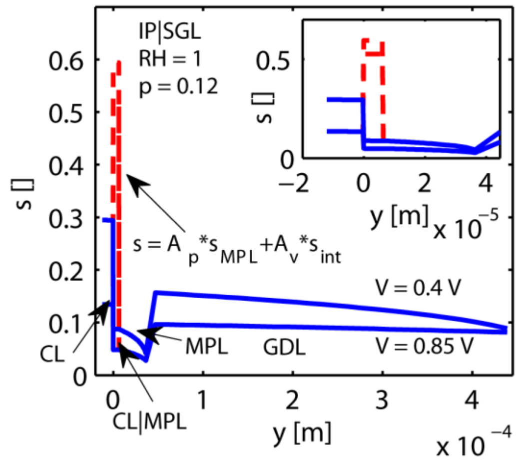

Figure 1: Through-plane saturation profiles for the PEFC including the IP|SGL interface at RH = 1 and p = 1 MPa for potentials of 0.4 and 0.85 V. The inset shows a zoom-in view of saturation profiles at the CL|MPL interface.

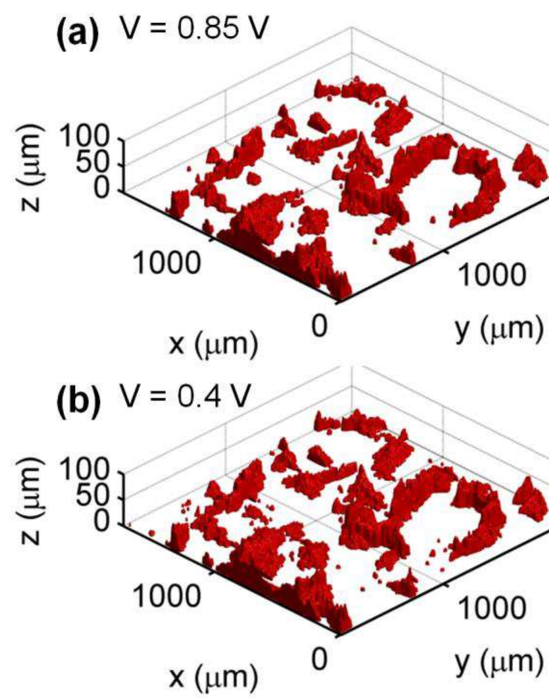

Figure 2: Three-dimensional water distribution profiles generated by deterministic contact mechanics model for compressed IP|SGL interface at (a) V = 0.85 V and (b) V = 0.4 V.

In this paper and presentation, we will outline the model's theory and present our investigations on the impact of the water accumulation and contact resistance at the CL|MPL interface on the PEFC performance.

REFERENCES

1. J. P. Owejan, T. A. Trabold, D. L. Jacobson, M. Arif and S. G. Kandlikar, Int. J. Hydrogen Energy, **32**, 4489 (2007).
2. Y. Aoyama, Kadowaki, K., Tabe, Y., Chikahisa, T., Observation of Water Transfer Phenomena in Micro-Porous Layer of PEFC, in ECS, ECS Transactions (2012).
3. I. V. Zenyuk, E. C. Kumbur and S. Litster, J. Power Sources. http://dx.doi.org/10.1016/j.jpowsour.2013.03.165