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Inhomogeneous assembly compression effects on two-phase transport phenomena in the anode of a DMFC

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A two-phase, isothermal, 2D/1D model is presented for the anode of a liquid-feed Direct Methanol Fuel Cell (DMFC). The model, which is an extension of the 3D/1D single-phase model previously proposed by Vera [1], takes into account the effects of anisotropic properties and inhomogeneous assembly compression of the Gas Diffusion Layer (GDL). The assembly process is simulated by a novel Finite Element Method (FEM) model, which fully incorporates the nonlineal orthotropic mechanical properties of the GDL [2]. The porosity distribution provided by this model is used to estimate the effective properties of the GDL, i.e. dry diffusivity, absolute permeability, capillary pressure and electrical conductivity, through empirical data reported in the open literature. The collected data corresponds to Toray® carbon paper TGP-H series. Multiphase transport is modeled according to the classical theory of porous media (two-fluid model), considering the effect of non-equilibrium evaporation and condensation of methanol and water.

The results show that GDL inhomogeneous compression may have a large impact on two-phase transport phenomena. The numerical results evidence that the hydrophobic Leverett J-function ($\theta_c > 90$º) is physically inconsistent to describe capillary transport in the anode of a DMFC. In contrast, more realistic results are obtained when experimental data reflecting the mixed-wettability characteristics of GDLs are taken into account. In particular, capillary transport in the anode of a DMFC seems to be better described by the capillary pressure curves associated to the drainage process (gas-phase displaces liquid-phase) as opposite to the hydrophobic Leverett J-function which predicts a similar behavior to that observed for GDL-specific imbibition curves (liquid-phase displaces gas-phase). As it can be seen in Fig. 1, due to the dominant role of the capillary pressure gradient in the gas-flow, the increasing negative capillary pressures ($p_c = p_g - p_l$) predicted by the hydrophobic Leverett J-function (GDL-specific imbibition data) as the GDL is compressed [3] results in an unrealistic reverse gas-flow towards the regions of lower porosity. In contrast, the increasing positive values of the capillary pressure associated with GDL-specific drainage data as the GDL is compressed [3] results in a more realistic gas-flow towards the regions of higher porosity, i.e., the virtually uncompressed region under the channel.

In addition, the numerical results show that the gas coverage factor at the GDL/channel interface may have a strong influence on the gas-void fraction distribution in the GDL. The parameter which governs the gas saturation distribution in the GDL is the ratio Γ, defined as the quotient between the partial derivative of the capillary pressure with respect to the porosity and with respect to the liquid saturation. This parameter measures the importance of the capillary resistance induced by the inhomogeneous compression (proportional to the partial derivative with respect to the porosity) as compared to the effect of the capillary diffusivity (proportional to the partial derivative with respect to the liquid saturation). As shown in Fig. 2, due to the particular shape of GDL-specific drainage curves [3], the influence of the capillary resistance results negligible, $\Gamma \ll 1$, when the gas saturation level in the GDL is small ($1 - s^{in} = 0$). In this situation, the gas saturation distribution is exclusively dominated by the effect of the capillary diffusivity and, therefore, a higher gas-void fraction results under the rib. However, for intermediate gas saturation levels the effect of the capillary resistance becomes comparable to the effect of the capillary diffusivity, $\Gamma \sim O(1)$, leading to a lower gas-void fraction in the regions where the porosity is also lower, i.e., the more compressed regions under the rib. In particular, the gas saturation decreases significantly in the region under the rib corner due to the sharp reduction of the porosity there. This singular region seems to be a preferential location for the evacuation of the gas phase bubbles from the GDL to the channel.

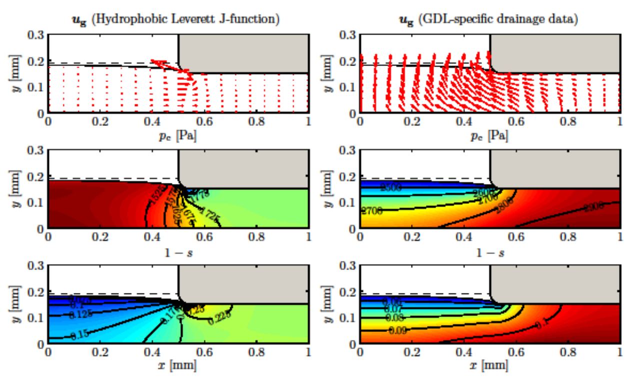

Fig. 1: Gas-phase velocity, $\mathbf{u}_g$, capillary pressure, p_c, and gas-void fraction, $1 - s$, as predicted by considering the hydrophobic Leverett J-function (θ_c = 100º) (left), and GDL-specific drainage data [3] (right). Operating Conditions: $V = 0.25$ V, CR (Compression Ratio) = 20%, $1-s^{in} = 0.95$, $C_{ml}^{in} = 1$M, $T = 80$ºC.

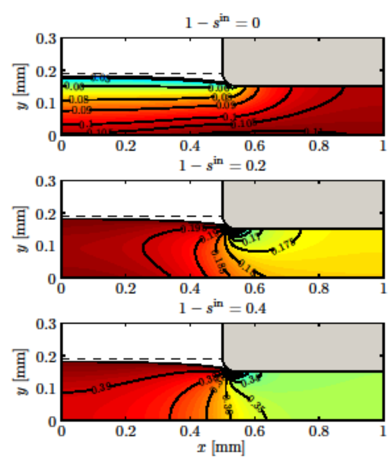

Fig. 2: Gas-void fraction, $1-s$, for different gas coverage factors at the GDL/channel interface, $1 - s^{in}$. Operating Conditions: $V = 0.2$ V, CR (Compression Ratio) = 20%, $C_{ml}^{in} = 1$M, $T = 80$ºC.

References

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[3] Gostick J.T., Ioannidis M.A., Fowler M.W., Pritzker M.D., J. Power Sources 194 (2009) 433-444.