Understanding invasion mechanisms in fibrous gas diffusion media: Direct comparison of simulations with tomographic visualization

Jeff T Gostick[1], Gisuk Hwang[2] and Adam Weber[2]

[1]McGill University, Montreal, QC, Canada
[2]Lawrence Berkeley National Lab, Berkeley, CA, USA

The movement of liquid water in the porous electrodes of polymer electrolyte fuel cells plays a decisive role in cell performance. The present understanding of multiphase flow in fuel cells has been limited by the general lack of experimental tools and theoretical models applicable to these nonconventional porous materials. Fuel cell electrodes and specifically the gas diffusion media (GDM) possess many atypical characteristics, such as neutral wettability, fibrous geometry, high porosity, finite size, and so on, that are not well described by the traditional porous materials toolset. For instance, the ubiquitous Washburn equation for relating the radius of a capillary tube to the capillary entry pressure fails to predict many of the observed capillary pressure characteristics, such as the lack of spontaneous imbibition of either water or air, regardless of any hydrophobic treatment (*1*). One of the defining characteristics of GDMs is their neutral wettability (*2*), which means that pore geometry plays an increased role in the capillary behavior (*3*). When this fact is coupled with their highly porous nature and fibrous solid structure, it is expected that the fluid invasion processes differ considerably (*4*) from the traditional picture of a highly non-wetting fluid injecting into a long, straight cylindrical capillary. In this work, the invasion patterns of fluids into fibrous GDM substrates were studied by several means to help understand and differentiate the impact of wettability and geometry.

Firstly, the micron-resolution X-ray tomography beamline at Lawrence Berkeley National Lab's Advanced Light Source was used to obtain 3D images of water injection into dry materials, as well as injection of air into samples filled with a perfectly wetting fluid. Phase contrast-based reconstruction was used (*5*) and high quality 3D images were obtained as shown in Figure 1. Using two fluids with highly different wettabilities makes it possible to deconvolute the impacts of wettability from pore geometry. The otherwise identical geometries mean that any significant differences in invasion patterns can be attributed to differences in the invasion mechanism owing to the large wettability differences.

To complement the direct experimental visualizations, simulations of fluid invasion were performed using a morphological image analysis approach similar to Hilpert and Miller (*6*) yielding invasion configurations as shown in Figure 2. This technique is commonly used in porous media research and has been previously applied to GDMs as well (*7*). This method assumes a perfectly wetting-nonwetting system (contact angle of 180^o), so it is comparable to the nonwetting fluid invasion images. This simulation technique has two key limitations: it neglects the aspect ratio of pore throats, and fails to handle menisci coalescence. Both of these limitations are especially relevant for fibrous GDMs, which have no discernible throat length (hence high likelihood of coalescence) and have an anisotropically oriented fibrous backbone (hence elongated throat shapes). Any deviations between the simulations and the images of nonwetting fluid invasion can be attributed to the atypical geometry of the GDM materials since the wettability is otherwise identical.

The ability to compare invasion configurations of two fluids with different wettability but otherwise identical geometry, and to compare fluids with identical wettability but that interact differently to the geometry will provide significant insights into the mechanisms of displacement in GDMs and other atypical porous materials.

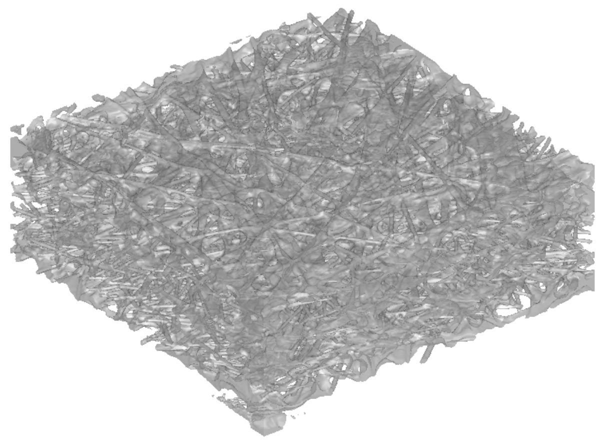

Figure 1: Reconstructed 3D image of dry Toray 120 (10wt% PTFE)

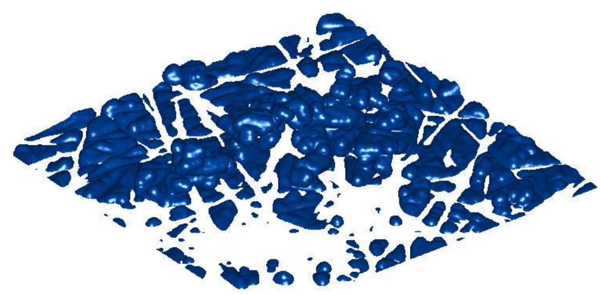

Figure 2: Simulated nonwetting fluid invasion configuration

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