ADVANCES IN DIGITAL MICROSTRUCTURE GENERATION OF A PEMFC GDL WITH LOCALIZED BINDER AND PTFE DISTRIBUTIONS

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ABSTRACT
In this work, a new framework and model for the digital generation and characterization of the microstructure of GDL materials with localized binder and polytetrafluoroethylene (PTFE) distributions were developed using 3D morphological imaging processing. This new generation technique closely mimics manufacturing processes and produces for the first time complete phase-differentiated (void, fiber, binder, and PTFE) digital 3D microstructures in a cost- and time-effective manner. The results for the digital generation of Toray TGP-H-060 with 5 and 0 wt.% PTFE were in close agreement with confocal laser scanning microscope (CLSM) images as well as 3D X-ray tomography studies. The resulting structure can be readily used for analyzing transport processes utilizing commercial CFD software.

INTRODUCTION
The ability of a gas diffusion layer (GDL) to efficiently provide the several vital functions in proton exchange membrane fuel cells (PEMFCs) is intrinsically linked to the microstructure geometry and its composition. Accurate information on the distributions of graphitized fiber, carbonized resin, and PTFE is highly desired. The direct measurement of these quantities remains prohibitively difficult and thus a modeling approach to digitally generate representative GDL microstructures is increasingly advantageous.

A relatively new method utilizing the field of stochastic geometry to predict the internal microstructure of GDL materials has proven to be a valuable tool to ascertain GDL 3D geometry and composition in a cost- and time-effective manner (1,2). Using this method, the GDL skeleton can be generated using a Poisson line process to represent the centers of the fibers. The binder has typically been generated by first classifying each voxel in the pore structure as a particular pore size and then the voxels belonging to the smallest pore sizes are filled until the desired percent binder is obtained (2). However, obtaining accurate distributions of both binder and PTFE is critical in modeling liquid water and reactant transport through GDL materials. For the first time, this work focuses on generating a comprehensive model with localized distributions of both components.

MODEL FOR GDL MICROSTRUCTURE
The graphitized fiber skeleton of a GDL was modeled as a random collection of cylinders uniquely defined by a unit vector Ĉ and a point \((x_0,y_0,z_0)\) it passes through. Randomization of the collection of digital fibers was achieved through the use of a pseudo-random number generator for both the orientation Ĉ and the point \((x_0,y_0,z_0)\) it passes through. To model highly anisotropic GDL materials, the through-plane component of Ĉ was suppressed and \(z_0\) points were selected such that the fiber skeleton was constructed by stacking layers until the desired thickness was obtained.

The carbonaceous binder in actual GDL materials is typically added as a thermoset resin during fabrication and behaves as a wetting fluid prior to carbonization (3). This behavior is evident in the CLSM images of Toray TGP-H-060 without PTFE treatment in Fig. 1a. The image shows the binder material retained the thermoset resin’s relatively low static contact angle on the fibers and generally accumulated at fiber intersections. This behavior was mimicked digitally by using 3D morphological image processing on the fiber skeleton. This newly developed method of adding the binder material to the fiber skeleton is representative of manufacturing techniques and provides a digital analogy to the physical interaction of the binder materials with the fibrous substrate.

Polytetrafluoroethylene is commonly added to GDL materials to increase hydrophobicity and improve water management (3). In this study, the PTFE treatment was
mimicked digitally using a second 3D morphological processing step on the GDL substrate.

RESULTS

A direct qualitative comparison of the generation algorithm to actual a GDL is made in Fig. 1 where Fig. 1a shows a CLSM image of Toray TGP-H-060 with 0 wt.% PTFE and Fig. 1b shows the digital GDL with grayscale representative of depth. Note from these images that the binder morphology produced using this method is in close agreement with actual Toray TGP-H-060. The converged porosity of the generation was determined to be 81 % with 30 % volume fraction of binder which is in good agreement with manufacturer data (4).

The generation algorithm was also compared to the actual 3D structure of Toray TGP-H-060 0 wt.% PTFE obtained by Becker et al. (2) using synchrotron-based phase contrast X-ray tomographic microscopy. The through-plane pore structure and binder-fiber interaction of actual Toray TGP-H-060 0 wt.% PTFE is shown in Fig. 2a (2) and Fig. 2b shows a similar cross-sectional slice of the digitally generated GDL. The areal density and binder-fibers interaction shown in these images are in close agreement indicating the model of the binder was representative of the 3D nature of actual GDL materials.

The generated 3D phase-differentiated (void, fiber, binder, and PTFE) microstructure allows for material characterization on any part or whole that may be unavailable otherwise. Figure 3 shows a central ½ µm slice of a generated GDL that simulates Toray TGP-H-060 5 wt.% PTFE with void, fiber, binder, and PTFE shown as black, green, orange, and cyan, respectively. These local variations in distribution of the phases in relation to the channel and land configuration in an actual PEMFC could have a strong effect on the local current density, water saturation, and temperature distribution and should be accounted for in modeling efforts.

CONCLUSIONS

A new framework and model were developed for the digital generation and characterization of the microstructure of GDL materials with localized binder and PTFE distributions. This numerical simulation tool closely mimicked manufacturing processes and for the first time produced realistic 3D phase-differentiated (void, fiber, binder, and PTFE) digital microstructures in a cost- and time-effective manner. The resulting structure can be readily used for analyzing transport processes by using commercial CFD software packages.

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REFERENCES

(4) Toray Industries, Inc. Manufacture data.