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OpenPNM: An Open Source Pore Network Modeling Framework for General Scientific Applications

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Pore network models (PNM) have been increasingly applied to study multiphase flow in the PEM fuel cell electrode in the past few years [1-10]. There are two principle reasons for this trend. Firstly, unlike the traditionally used continuum models, PNMs do not require constitutive relationships for multiphase transport properties, such as relative permeability and effective diffusivity, which are very difficult to measure reliably. In fact, PNMs are able to predict transport properties as a function of porous structure (i.e. porosity, anisotropy, pore sizes). Secondly, continuum models do not resolve the discrete liquid configurations in the electrode, so the fail to predict many important effects. For instance, the presence of liquid clusters in the GDL leads localized regions of near-infinite diffusion resistance, while continuum models reduce diffusivity as a gradual function of volume averaged water content. Moreover, continuum models predict liquid water profiles in the GDL that are in stark contrast to those observed in x-ray tomography experiments and pore network models.

Despite these limitations, continuum models continue to see wide spread use. This is at least in part due to the numerous user-friendly software packages that are commercially available. PNMs on the other hand, are usually developed from scratch by individual research groups. There is clearly a need for a generalized, flexible software distribution to help ease the adoption of this powerful and useful paradigm. This presentation will introduce a collaborative software development effort spearheaded by AFCC and Ford, in conjunction with two academic labs both involved in the PNM field. The result is a package named OpenPNM that is designed to be shared with interested researchers as free, open source software. The package is written in Python and will available for download from OpenPNM.org.

The current version of OpenPNM possesses the basic set of PNM capabilities (capillary pressure curves, multiphase transport calculations, etc), with additional complexity to be added progressively in future releases. The software was written using an object-oriented architecture to facilitate modularity, extensibility and customization. The standard network generation produces a regular cubic lattice, though the framework is general enough to accommodate any topology. This enables the user to import any topology (e.g. from extracted networks) and utilize the OpenPNM toolset directly.

Figure 1 shows an invasion pattern into a 40 x 40 x 20 pore network according to the invasion percolation algorithm. The pores are colored according to their invasion sequence, and the invasion was halted when a pore on the outlet face was invaded. Figure 2 shows an oxygen concentration profile in a dry network with Dirichlet boundary conditions of x_{oxygen} = 0.5 and 0.05 on the top and bottom of the domain respectively.

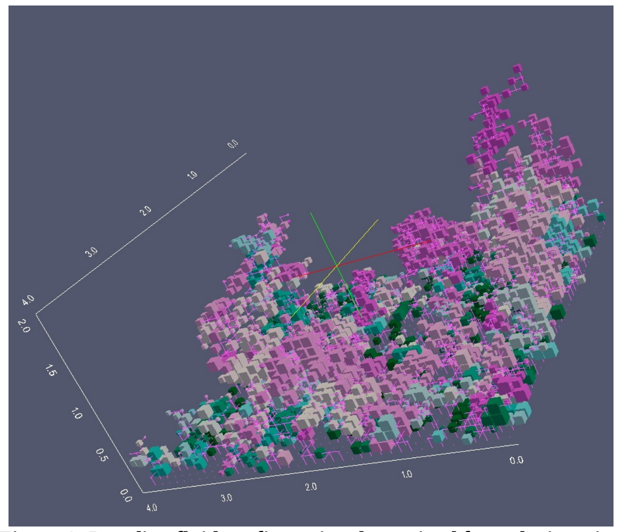

Figure 1: Invading fluid configuration determined from the invasion percolation algorithm.

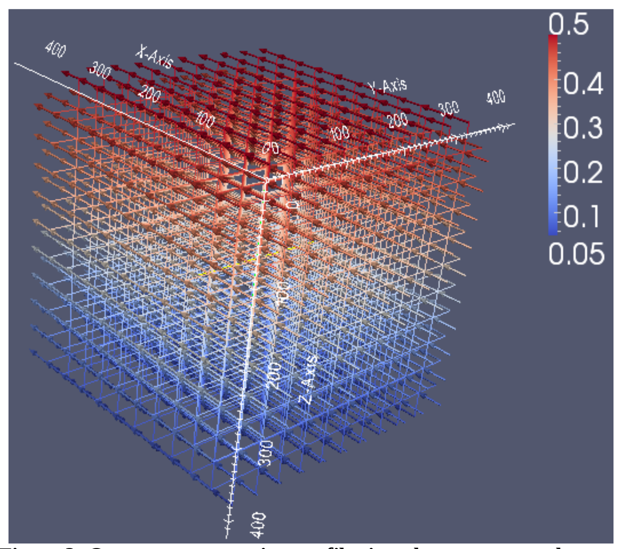

Figure 2: Oxygen concentration profiles in a dry pore network.

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