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Modeling of composite fibrous porous diffusion media

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ABSTRACT

To engineer the desired properties of fibrous porous media, a parametric modeling approach is needed to support the rational design of the materials before the fabrication. In this study, we propose a methodology that enables the accurate representation of three-dimensional (3D) microstructures of fibrous porous media and prediction of their transport properties. Toray TGP-H-060 gas diffusion layer (GDL) is selected as an example to demonstrate the feasibility of the suggested design methodology. The detailed microstructure of the GDL with the inclusion of locally distributed binder is constructed using an extended periodic surface (PS) modeling technique. A 3D morphological approach is taken to create the binder distribution within the fibrous microstructure. Transport properties including permeability, relative diffusivity, and tortuosity and local structure characteristics of the generated microstructure, under different binder loading are calculated. It is shown that the detailed model of the fiber-binder composite has a strong influence on the predicted properties.

Introduction

Fibrous porous media have been used for many decades in a plethora of industries such as bioengineering, electronics, energy and environmental processes [1–6]. As an example, gas diffusion layers (GDL) are used in polymer electrolyte membrane fuel cells (PEMFC), a burgeoning renewable energy resource. GDLs serve as electrodes in PEMFCs, which permeate gases and help remove water droplets that are formed during fuel cell operation. Furthermore, these carbon based GDLs have other properties such as high porosity, strength-to-weight ratio, and electrical and thermal conductivities that make them attractive for use in PEMFCs and other areas [7].

It has been shown that the performance of PEMFCs depends upon the morphological, transport, and mechanical properties of the GDLs [8–12]. However, no systematic and parametric modeling approach that help predict and optimize the key characteristics of porous materials such as GDLs for the purpose of materials design exists to date [13]. Rather, studies have been conducted to determine the morphological and transport properties of the fibrous diffusion media that have been fabricated [14]. In these studies, the microstructure of the porous media was generated by image-based reconstruction or geometrical construction approaches. In the

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image-based approaches, 2D images or 3D voxel representation of the internal pore structures are obtained by scanning electron microscopy (SEM), synchrotron-based tomography, confocal microscopy, or computed microtomography (μCT) [15–24]. Although imaging techniques accurately capture the geometry of porous structures, the model of the microstructures reconstructed from the images cannot be modified. Thus, imaged-based approaches are not suitable for designing microstructures of porous media. The geometrical construction approaches that utilize conventional computer aided design (CAD) tools are not efficient in modeling complex structures. Because in these approaches, a large number of discrete control points are required to accurately represent the topology of the porous media. Conversely, implicit surface modeling approaches that construct the microstructures based on closed-form mathematical functions are much more promising [25].

The geometrical construction of fibrous diffusion media has been primarily based on statistical methods. Fibers are assumed to have simple shapes such as long cylinders and randomly distributed in a representative volume element (RVE). In the work of Schulz et al. [26], the fiber skeleton of GDLs was modeled as a collection of intersecting cylinders oriented along randomly distributed axes. The directional distribution of the fibers was assumed as normal or determined from the SEM images. Thiedmann et al. [24] constructed GDL microstructures by implementing a Poisson planar line tessellations (PLT) process to represent the fibers' axes. Gaiselmann et al. [27] represented the pore space of fibrous media with random geometric graphs. The parameters required for modeling were specified such that the distributions of vertex degrees and edge lengths conform with X-ray synchrotron tomography images. GDLs have also been represented with simplified geometries such as arrays of parallel and perpendicular cylinders or channels [28,29].

Fibrous porous media are often more complex than a collection of fibers. They also include some binding material(s). To model the binder in the microstructure of the GDL, the pore space of the generated fiber skeleton is filled using various approaches such as stochastic methods with predefined probability functions or morphological operations [24,30].

To quantitatively characterize the pore space of a porous medium and to predict its bulk material properties, the morphological properties of the generated microstructure (e.g., pore size and shortest path distributions) have been also studied. The pore size has been calculated as the spherical distance of the points inside the void space to the surrounding solid boundaries [31–33]. However, in some studies, the pores were defined as 2D closed areas and the pore size is defined as the diameter of a circle with an area equal to the closed area [34,35]. To determine the inhomogeneity and directionality of the distribution of pores in the microstructure, the chord length distribution of a porous medium was also found by evaluating angularly resolved lineal path functions [36]. The distribution of the shortest path within a porous microstructure has been found from the voxel mesh or the graph representation of the porous domain [24,36], using Dijkstra's algorithm [37]. The existing numerical schemes offer useful platforms and tools for the evaluation of some morphological properties. However, they are computationally expensive. In the current study, these schemes are modified for higher accuracy and lower computational time.

Transport properties of microstructures can be predicted using different approaches such as pore network (PN), lattice Boltzmann models (LBM) and computational fluid dynamics (CFD). The effects of change in porosity due to the compression forces and fiber size and spatial orientation have been investigated through permeability, tortuosity, diffusion and relative permeability of fibrous porous media [14]. The CFD approach is more time efficient than LBM and can simulate larger domains. The PN modeling approach uses a simplified representation of the pore structure and is efficient for large domains. However, it requires the information of length correlations that need to be extracted from an existing structure. The process itself is time consuming.

The objective of this work is to introduce a platform for designing composite porous media, with the characteristics that are similar to those of GDLs. A new methodology is developed to generate the fiber skeleton of composite porous diffusion media. In this study, a periodic surface (PS) modeling technique developed by Wang [25] is used to generate the fibrous component of the microstructures, and the binder distribution is modeled by the Minkowski sum of fibers and a structure element (SE). The microstructure generation process is directly integrated with the morphology and transport characterization analyses.

Material

Toray TGP-H-060 carbon paper GDL, shown in Fig. 1, is chosen as the fibrous composite microstructure to examine the feasibility of the microstructure generation method. Toray TGP 060 is made of a matrix of carbonaceous binder that is a thermoset resin and graphitized rigid carbon fibers [22]. Typical parameters of the GDL include, a fiber diameter of 7 μm, a thickness of 200 μm, porosity of 0.78 and 0.27 solid fraction of carbonaceous thermoset binder [30].

Implicit surface modeling of fibrous structures

An implicit surface $S = \{r \in \mathbf{R}^3 : \psi(r) = 0\}$ is defined as a set of points that are the roots of a given function $\psi : \mathbf{R}^3 \rightarrow \mathbf{R}$ with real-valued coordinates. Recently a periodic surface (PS) model was developed by Wang [25] to implicitly model structures with complex topology, which is define as

$$\psi(r) = \sum_{l=1}^{L} \sum_{m=1}^{M} \mu_{lm} \cos\left(2\pi\kappa_l \left(\mathbf{P}_m^{\mathrm{T}} \cdot \mathbf{r}\right)\right) = 0 \quad (1)$$

where $\psi(r)$ is the implicit function, μ_{lm} is periodic moment, κ_l is the scale parameter, $\mathbf{P}_\mathrm{m} = [a_m, b_m, c_m, \alpha_m]^\mathrm{T}$ is a basis vector for the major phase, $[a_m, b_m, c_m]^\mathrm{T}$ represents the normal vector of the basis plane, α_m is the phase of the plane, $\mathbf{r} = [x, y, z, 1]^\mathrm{T}$ is the location vector in homogenous coordinates. The PS model of a rod surface with the periodicity of 1 along the z-axis direction in an RVE is: