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Modeling of gas diffusion layers with curved fibers using a genetic algorithm

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ABSTRACT

This paper presents a methodology for modeling microstructures of fibrous porous media with curved fibers. The developed methodology utilizes implicit periodic surface model coupled with the genetic algorithm (GA) optimization to construct the porous microstructures. The fibers profile is represented by the periodic implicit surfaces and their orientation and curvature are determined by GA optimization. To reconstruct the microstructures with higher resemblance to the actual porous media GA is utilized to minimize the fibers stored strain energy and their intersection volumes. Coupling the image processing techniques to the geometry construction procedure the morphological and transport properties of the constructed microstructures are also determined. To verify the feasibility and the accuracy of the proposed methodology the microstructure of Freudenberg H2315 GDL is constructed and characterized. The presented methodology enables a parametric design approach. Thus, the effects of the microstructure's properties e.g., fibers diameter, fibers orientation and porosity of the porous structure on the transport properties of the fibrous media are investigated.

Introduction

Fibrous media have extensive applications in various industries such as renewable energy, transportation, and bioengineering. They are found in woven and nonwoven forms. The nonwoven media are manufactured as paper or felt structures. In the paper media fibers are usually straight and are bonded together in a matrix of resin. The resin increases the delamination resistance and mechanical strength against shear forces. The felt structures are usually manufactured by carding the fibers using hydrogentanglement. In the thin fleece manufactured by this method fibers are mechanically bonded, curved and entangled in the through plane direction [1,2].

The properties of the porous media affect the overall performance of the systems utilizing them. As an example, the performance of polymer electrolyte membrane fuel cells (PEMFCs) depends on the functionality of their fibrous media known as gas diffusion layers (GDLs). GDLs are carbon base porous media with several functionalities, such as transport of the reactant gasses, electronic conductivity and mechanical support [3]. It has been found that the morphological and transport properties of the GDLs have large impact on the performance of the fuel cells. Since, there is a correlation between the GDL's microstructure and the limiting current

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density of the PEMFCs, accurate reconstruction and characterization methods are necessary [4].

Various characterization and modeling approaches have been implemented to determine the morphological and transport properties of the fibrous media. Destructive and non-destructive imaging techniques such as micro and nano scale computed tomography (μCT) and confocal microscopy [5–9] were used to inspect and construct the microstructure of porous media. Fishman et al. [10] used μCT to determine the porosity distribution in the woven and nonwoven GDLs. Becker et al. [11] used μCT imaging to investigate the variation of GDL's microstructure under compression. Banerjee et al. [12] developed a new segmentation methodology to capture X-ray images of GDL with a micro porous layer. The suggested segmentation methodology is based on the areal mass and volume of the GDL and is capable of generating repeatable multicomponent segmentation. Cooper et al. [13] used neutron radiography to determine the water distribution in a working fuel cell. They investigated the effect of permeability on water saturation of various types of GDLs and determined their optimal operating condition. A variety of geometrical modeling techniques have been also suggested for modeling woven and nonwoven fibrous structures. The woven structures have been often modeled using CAD tools such as, non-uniform rational B-spline (NURBS), commercial CAD software packages. Their microstructures were constructed by building the central axis of the yarn and sweeping the cross sections [14–18].

In the nonwoven porous media positions of the fibers are undetermined. So, random models have been usually implemented to construct their microstructures. SEM images were used to determine the random distribution of fibers in a representative volume element (RVE) [19–21]. Hinebaugh et al. [22] used various imaging methodologies such as optical microscopy, SEM and computed tomography to characterize seven commercially available GDLs and measured the diameter, alignment and area density of fibers, in addition to the size of the cracks in the micro porous layer. Using this metadata from various type of GDLs Hinebaugh et al. [23] developed a stochastic modeling methodology for virtual reconstruction of GDL RVEs. In the RVEs the volume fraction of binder, fibers diameter and alignments were also modeled using the collected metadata. Schulz et al. [21] presented a layered 3D model of a GDL, assuming infinitely long fibers in the form of cylinders with a priori spatial distribution function. Mukherjee et al. [24] and Inoue et al. [25] also applied stochastic reconstruction methods similar to that proposed by Schulz et al. to construct the GDLs. Thiedmann et al. [26] constructed the GDL microstructures assuming a layered structure and implementing a planar random line tessellations (PLT) process. To model the composite structure of papers, the fibrous skeleton was generated using statistical models. The binder was modeled by filling the pore space with various types of fillers such as thin sheets and spherical elements [26,27]. Daino et al. [27] generated the fibrous skeleton of the GDL using the statistical models and implemented morphological filling to model the binder in the pore spaces. Zamel et al. [28] modeled the composite structure of the GDL including micro porous layer using stochastic methods. To model the microstructures of the felt media Gaiselmann et al. [29] reconstructed the curved fibers of the felt GDL. They assumed that felt GDL is composed of a stack of thin sheets with horizontally distributed fibers. The distribution of fibers was determined by a 3D geometric graph extracted from the SEM images.

To study the effects of the fibrous structures on the system performance, the microstructures constructed by imaging methods or geometrical models need to be further studied. The morphological, mechanical and transport properties of the fibrous structures are the properties of interest. Morphological property of the porous media is defined by their pore size distribution, pore connectivity, chord lengths and tortuosity. Commonly, a pore is defined as the spherical available distance inside the void space of the porous media. Thiedmann et al. found the pore size distribution of a GDL from its graph representation. They defined a pore as the largest sphere fitted in the pore space with three contact points with the solid phase [26,30,31]. The numerical pore size distributions were compared against the pore size distribution determined from mercury intrusion porosimetry (MIP) tests. Since the dead-end pores and the pores not connected in the through-plane direction are not accessible in the MIP, these pores were excluded from the pore size distribution [32]. To account for the inhomogeneity of the fibrous structures the chord length distributions in the through plane and in plane directions have been determined [33,34]. To study the effect of the morphology of the fibrous media on their transport properties the distribution of the shortest paths has been also studied [30,33,35]. For this purpose, a graph representation of the porous medium is constructed and a search algorithm is then implemented to find the shortest possible path from the vertices on the inlet to any of the vertices located at the designated exit [36]. Using a similar approach, Gaiselmann et al. found the shortest path distribution of a virtual representation of felt GDL [29].

To determine the transport properties of the reconstructed fibrous media pore network modeling [24,37–40], lattice Boltzmann [41–44] and computational fluid dynamic (CFD) [45] approaches have been implemented and the transport properties such as fluid tortuosity, permeability and diffusivity of the porous media have been computed. Software packages such as Simpleware [46] and Geo-Dict [32] have been developed that determine the transport properties of the reconstructed RVE of the fibrous media. The Geo-Dict software also enables the reconstruction of the fibrous microstructures as well as characterization of the RVEs [32]. Froning et al. [47] generated the geometry of the felt GDL using the stochastic model suggested by Gaiselmann et al. [47]. They computed the permeability of the reconstructed microstructure using lattice Boltzmann simulations and investigated the effect of compression on the GDLs transport properties.

To support the multi scale modeling attribute needed for modeling porous structures with nano and micro scale features Wang [48] introduced periodic implicit surface (PS) model. PS models are closed form mathematical functions developed to represent features of porous media. Huang et al. [49] introduced PS models of different types of fibers observed in the porous media, e.g., straight, bent and curved fibers. Didari et al. developed a methodology to construct the microstructure of paper media using the straight fibers' PS

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