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3D stochastic modeling, simulation and analysis of effective thermal conductivity in fibrous media

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ABSTRACT

This paper develops a 3D stochastic model to describe porous metal fiber sintered sheet (PMFSS), which is a non-woven fiber mat composed of curved and partial overlapped sintered fibers. Firstly, single fibers of PMFSS are modeled based on morphology information involving curvature and orientation extracted from the actual structure employing the 3D micro-CT imaging. Secondly, since fibers are partially overlapped at sintered joints (fiber to fiber overlapping section) during sheet formation process, a graphics processing unit (GPU) accelerated force biased simulation is introduced, which turns the arbitrarily overlapped single fibers into partially overlapped ones, for the sake of making the virtual geometry more realistic. Finally, fibrous geometries resembling the microstructure of PMFSS with various porosities are established and further imported into the STAR-CCM+ CFD package (CD-adapco, London) to study the effective thermal conductivity. Results illustrate that the numerical effective thermal conductivity of PMFSS agrees well with the experimental results in the in-plane direction. Besides, the sensitiveness of effective thermal conductivity due to structural anisotropy is also verified.

1. Introduction

In recent years, fibrous porous materials, such as the porous metal fiber sintered sheet (PMFSS), have attracted considerable attention in engineering areas due to their outstanding mechanical and transport properties. PMFSS has been successfully applied to the fuel cell as micro-channel [1] to increase the contact area during the reaction. Furthermore, it is expanded for using in loop heat pipe as wick structure [2], where accurate determination of the heat transfer is essential for the operation and design of the system.

PMFSS is composed of arbitrarily curve fibers. These fibers are bonded together during sintering process and finally, a complex network system is generated, which contributes to its enhanced properties. Different techniques have been applied to characterize the fibrous porous structure and transport properties. Sadeghi et al. [3] developed a compact analytical model for evaluating the effective thermal conductivity of fibrous gas diffusion layer (GDL). Their geometrical model was an idealization of actual material consisted of uniformly sized equally spaced cylindrical fibers. Zamel et al. [4] developed digitally stochastic models of carbon paper, the fibers were considered to be cylindrical and arbitrarily overlapped, the orientation of fibers was determined by a one-parametric directional distribution to ensure that the fibers were isotropic in the in-plane direction and anisotropic in the through-plane direction. To control the extent of fiber-to-fiber interpenetration and capture its structural effect on heat conduction simulation, Arambakam et al. [5] placed a restriction on the allowable distance between the axes of two straight fibers at their crossover points.

Besides analytical and numerical measurements, experimental approaches have also been proposed to measure the thermal conductivity of fibrous porous media. Li et al. [7] designed an experimental apparatus to measure the effective thermal conductivity of porous stainless steel fiber felt, the contribution of three mechanisms to the total thermal conductivity, involving matrix heat conduction, air natural convection, and matrix thermal radiation, were evaluated. Sadeghi et al. [8] studied the heat transfer through the gas diffusion layer (GDL). A test bed that allowed separation of in-plane effective thermal conductivity and thermal contact resistance in GDL was described. The measurements were compared with a compact analytical model and good agreement was achieved.

As revealed in above literature, the effects of the fibrous porous microstructure on the macroscopic properties have been investigated from the analytical [3,8,9], numerical [4–6] and experimental [7,8,10] approaches. Both experimental and theoretical studies have revealed

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that the microstructure features significantly affect the thermal conductivity. However, it should be pointed out that it's difficult and time consuming to sensitively capture the impact of tiny microstructural alteration by the experimental data. In addition, the limitation of analytical or theoretical approaches is attribute to the simplified and idealized geometry models. To the best of the author's knowledge, the numerical studies of transport or mechanical properties of fibrous media were less reported than other numerical results, such as permeability and diffusion among the void phase. The main challenge is that more accurate representation of microstructure, especially fiber curvature and fiber-to-fiber crossovers, is required to estimate the solid phase transport properties.

Therefore, the computational fibrous material design has been the focus of many recent studies. More precisely, through establishing realistic stochastic models and taking into account the morphology variability introduced by varying manufacture factors, the correlation between microstructure and transport property can be evaluated and the microstructure with the best simulation performance can be detected.

Recently, there are several models of non-woven fibrous materials which consist of straight [3–5] or curved [11–13] fibers. As aforementioned, although many models are proposed, seldom of them is reported composed of both curved and overlapping controllable fibers. Even though the distance of axes of two straight fibers can be directly determined, however, as the number of fibers increases, the efficiency of modeling turns slow significantly. Additionally, the solid volume fraction (SVF, equivalent to 1-porosity) is limited in models composed of straight and non-overlapping fibers.

To mimic fibrous porous media composed of curved and non-overlapping fibers, Gaislemann et al. [11] introduced a stochastic 3D model, single fibers in GDL were described in terms of multivariate time series. The random fiber system was then transformed into a system of non-overlapping fibers using a force-biased collision detection algorithm proposed by Altendorf and Jeulin [12]. The principle of the force-biased algorithm is to represent single fibers as a chain of balls with the ball centers located in the centerline of each fiber. Then, a mass-spring force system was employed to simulate the collision between the ball-chain representing fibers and additionally, an angle force was introduced to preserve the local structure (curvature) of each fiber. For computational efficiency, the fiber system was subdivided into small regions and parallel performed to accelerate the computing.

Venkateshan et al. [14] proposed an approximate mass-spring-damper model to simulate the deformation of fibers to the geometry on which they deposited. To make the collision detection simulation more efficiently, the ball-chain representing straight fibers were added and simulated to the fiber system one by one. Additionally, only a sub-list of balls in fiber was processed during collision detection simulation for the computing efficiency.

It is clear that the computing cost is an important issue for the simulation of ball chain system. Thus, in the present paper, a GPU accelerated 3D stochastic model composed of curved and partial overlapping fibers is proposed. Firstly, Single fibers are represented with morphological statistics data involving orientation and curvature of traced single fibers employing Micro-CT technic, and a prime fiber system is generated as an assembly of these arbitrary overlapping fibers. Then, a GPU accelerated collision detection algorithm is proposed to transform the overlapping fiber system into a partial overlapping one to present the fiber-to-fiber sintered joints properly. Finally, the structure is validated via a good agreement between the numeral effective thermal conductivity and the experimental measurement. Furthermore, the impact of structural anisotropy on the transport property is verified.

2. Model description

2.1. Tracing of single fiber from 3D tomographic data

The virtual model is constructed based on the understanding of the microstructural characteristics of actual materials. The morphological features of PMFSS have been studied in our previous work [15], where various microstructural data are obtained based on the morphological analysis of the extracted skeleton (centerline) segments using micro-CT. However, the virtual modeling of fiber network requires quantitative morphology characterization of single fibers, rather than the fiber segments divided by fiber to fiber crossover (e.g., fiber joints at sintering regions in PMFSS). Therefore, a fiber tracing algorithm is described in details in our recent effort [16]. Briefly, single fibers are traced and connected by consecutively linking neighbor skeleton segments that show the most similar orientation and radius. Additionally, to reduce the misconnection due to the tracing orders, a multilevel tracing strategy is introduced. Subsequently, the quantitative morphology data involving distributions of orientation and tortuosity are obtained according to the traced single fibers. These data will be referred for model fitting in this work.

2.2. Prime overlapping modeling

2.2.1. Virtual curve single fiber with fitting curvature

The principle of single fiber modeling is to describe the fiber course by a spline curve, a geometric module integrated into software, e.g., MATLAB, SOLIDWORKS, etc. Firstly, several points are picked along the voxel-centerline (skeleton) of a single fiber at fixed interval using the 3D tomographic image. More precisely, the straight-line distance between two neighboring picked points is set as 100 voxels (the 3D image resolution is 9.4 μm per voxel). The length of the interval is moderately determined so that it can reflect the curvature without being oversampled or oversimplified in the modeling domain. Subsequently, these chosen voxels are connected with a straight line and the course of the fiber turns into a polygonal track $p=(p_0, p_1, \ldots, p_n)$. The polygonal track is then converted into a sequence of vectors $\{\vec{v}_i, i=0, \ldots, n-1\}$, with $\vec{v}_i$ composed of three components(l_i, θ_i, ϕ_i), where l_i represents the vector length, which is fixed in our case and θ_i (ϕ_i) denotes the change of direction azimuthal (polar) from $\vec{v}_{i-1}$ to $\vec{v}_i$ (Fig. 1). Compared with θ angle which represents the change of direction in the xy-plane (in-plane), the change of ϕ angle is very small. Thus, to simplify the modeling process and have a better control of the global through-thickness fiber orientation, single fibers are firstly modeled horizontally in the xy-plane with control points only considering the changes of directions (θ angle). The details of single fiber modeling are as follows,

1. Point p_0 is set at the origin point (0,0,0).
2. Orientation of vector $\vec{v}_0$ is randomly distributed in the interval [0,2π] in the xy-plane.

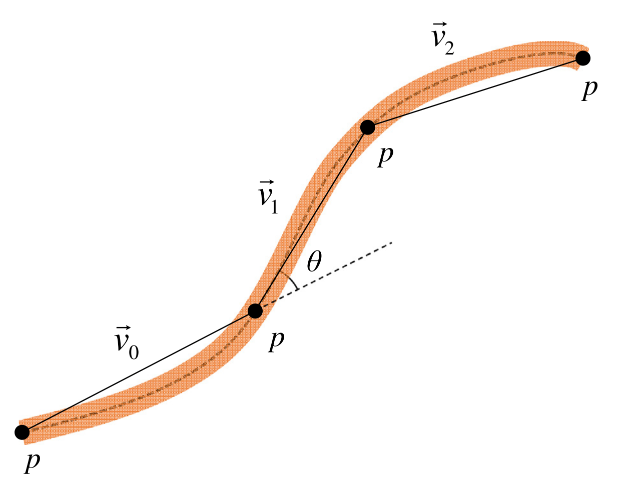

Fig. 1. Illustration of curved fiber represented as spline line.