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A new approach to digital generation of spherical void phase porous media microstructures

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ABSTRACT

This work describes a novel approach for obtaining digital samples of porous media based on a statistical knowledge of the microstructure of interest. The present formulation introduces a contact law based on bubble physics that is capable of handling interferences among spherical primitives of different diameter placed in a representative elemental volume, while the volume is compressed to yield a target porosity. The result is a statistically accurate mathematical model of a permeable, spherical-void-phase porous material that has the added feature of being spatially periodic in all principal directions. To validate the approach, digital samples of spherical-void-phase carbon foam were generated and discretized for use in hydraulic and thermal Computational Fluid Dynamics simulations. Relevant transport properties were computed from the simulation results, and compared to similar data found in the literature.

1. Introduction

Porous materials play an important role in many applications including heat pipes, heat sinks, automotive cooling devices and solar collectors. Any porous microstructure may be characterized by the statistical geometric properties: mean pore diameter, ligament length, surface area per unit volume, void shape, and geometric order, each of which might be correlated with changes in bulk material properties. The microstructural properties also affect exchanges that occur between fluid and solid phases in the case of flow through a permeable porous material, or in the case of external exposure to incident radiation. This has inspired many researchers to study the effects of pore structure variation on bulk material properties by developing representative, or idealized, geometric models. Such models permit analysis of properties and exchanges at the pore level, which can then be used to develop accurate mathematical models at the porous-continuum or volume-averaged level, which is what is used in most engineering analyses to deal with porous materials. In this paper, our interest is to develop a geometric model for spherical-void-phase (SVP) carbon foam that can be used to study exchanges that occur in a highly concentrated solar collector. Our interest in graphitic foam is that it is highly permeable, highly conductive and it has a high surface area to volume ratio. While pore-level geometric models do exist for spherical void phase materials, no current model is suitable to yield the material properties and exchanges, while preserving the random nature of the structure, which is required for consideration of radiation effects.

Currently, there are three main approaches to obtain bulk material properties, given the porous material of interest. First, experiments can be conducted to empirically determine the desired properties. While this method is quite useful for determining properties that can be used in engineering calculations, it can be difficult for researchers to understand the influence of the microstructure on the determined properties. Moreover, because experiments can only be performed on physical samples, the range of microstructures that can be studied is limited by current production capabilities.

The second method is to conduct Computer Tomography (CT) scans of a representative sample of the microstructure, thereby obtaining a digital representation of the structure. The raw data from the scan is post-processed to obtain a Computer-Aided Design (CAD) model. This model can then be used in computer simulations to determine the desired transport properties. Researchers including Haussener et al. [1], Maruyama et al. [2], and Anghelescu [3] have used this approach with some success. Unlike the experimental approach, this method allows researchers to visualize transport quantities and gradients throughout the pore level domain. However, the cost and accessibility of CT scanning equipment as well as the limitation of porous media production capabilities leaves more to be desired.

The final method is to generate a large number of small primitive objects (primitives) within a finite domain, where the

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dimensions of the primitives are decided based on statistical data describing the microstructure of interest. The interference of these primitives gives rise to the interesting features present in the porous domain. A finite volume filled with interfering primitives is thought to be an accurate representation of the desired microstructure. These digital domains can then be used in small-scale simulations to predict effective material properties. This method is unique in the fact that it does not require any physical representation of the domain, but only a statistical knowledge of the micro-structural features. Because this method deals with idealized representations of porous media, it is important to judge the relevance of all microstructural features to the bulk property of interest. Identifying which microstructural features whose variation does not influence a bulk property may allow a much simpler geometric model to be used. A first attempt by Yu et al. [4] constitutes the use of a simple primitive: the Boolean subtraction of a sphere from a cube (where the centroids of the sphere and cube are coincident). This primitive is stacked along all major axis to obtain a uniform structure of interconnected pores. This so-called unit-cube model is easy to generate and analyze digitally, however it does not capture the effect of bubble size variation, and it exhibits uncharacteristic properties due to the axis alignment of the bubbles. When used for studying trends in convective/conductive heat transfer and fluid flow, the unit cube model is sufficient, as predictions of permeability, inertial drag coefficients, and Nusselt number correlations were shown to be reasonable when the flow direction was oriented 45° from all principle planes [4,5]. Kumar et al. [6] performed Computational Fluid Dynamics (CFD) analyses involving the periodic tetrakaidecahedron structure (Kelvin cell) relevant to open-cell foams. The CFD results were compared with experimental results obtained using a uniform microstructure, which yielded excellent agreement. Leong and Li [7] determined the effective thermal conductivity of a unit cell which may be described as the Boolean subtraction of eight spheres from a cubic shell, where the spheres are centered on the vertices of the cube. James et al. [8] presented a novel approach for the generation of spherical-void phase (SVP) porous media wherein bubble diameters and interferences are chosen based on known probability distribution functions. That said, the method presented in [8] has some drawbacks, including the unrealistic assumption that the interference between two bubbles in contact is independent of their radii, and the random deletion of bubbles to obtain the desired porosity. In another work by Kırca et al. [9], carbon foam was modeled by selecting random points within a cubic domain as the sphere centers, and calculating the radii of the bubbles based on the desired porosity and the average bubble diameter. The method also suffered from the fact that bubble interferences were not determined. Wang and Pan [10] have proposed a random-generation growth method, wherein representations of open-cell foams are generated by randomly placing points in a 3D domain and stochastically linking neighboring nodes. Finally, in a recent publication by Chueh et al. [11], SVP was modeled by packing spheres into a periodic domain using the drop-and-roll method introduced by Visscher and Bolsterli [12]. This method relies on the assumption that bubble interferences can be prescribed using a constant contact angle, and periodicity is only enforced in two directions.

The primary motivation for developing the present method is to obtain digital samples of SVP carbon foam suitable for prediction of radiation transport properties. The ordered nature of the unit-cube model makes it a poor candidate for ray-tracing methods, such as that presented by Tancrez and Taine [13], so more accurate representations of SVP porous media are sought. In this work, the approach taken is similar to previous efforts, however in the Representative Elemental Volumes (REVs) produced using the current method, the interferences between features are governed by physically-based force–displacement relationship, and the REVs have the distinct advantage of being fully spatially periodic. The resulting models are then shown to produce the correct trends for pressure drop and convective heat transfer, thereby satisfying the necessary condition that fluid–solid interactions within the REV are properly predicted. Combined with the advantages of including variable pore size and preserving the random nature of the structure, the present modeling approach is considered most viable for studies on incident radiation.

2. Formulation

In the current approach, a 3D porous structure is generated from aggregate statistical data. For example, an isotropic SVP porous medium may have a statistical data set including an average bubble diameter and the standard deviation of the bubble diameters.

Once these data are determined, the method can be executed with the following steps:

(1) Select an Initial Volume (IV) shape and size. The IV should be large enough to completely envelop all of the geometric primitives without any of the primitives coming into contact with each other.
(2) Generate primitives. Choose the shape and dimensions of each primitive using a probabilistic model that reflects the statistical data. Then attempt to randomly locate each primitive within the IV, optionally choosing an orientation based on statistical data. If a primitive interferes with an already placed primitive, randomly select new locations and orientations until it does not interfere with other primitives. If a primitive cannot be placed after a large number of attempts, this may indicate that the IV is too small, in which case the algorithm should be restarted with a larger IV. The stopping criterion is at the discretion of the user. A simple approach is to stop after a pre-determined number of primitives have been placed.
(3) Using a Discrete Element Method (DEM) code, incrementally compress the IV over a sequence of time-steps. During each time-step, the domain boundaries are moved closer together. If the boundaries are chosen to be rigid walls, the primitives in contact with the boundaries will be forced inward, and come into contact with other primitives. Reaction forces (or separating forces) between primitives in contact are calculated using an appropriate force–displacement relationship, also known as a contact law. Eventually the primitives will reach a "jammed" state, where every primitive is locked in place. After the jammed state has been reached, further compression steps require ever-increasing forces to be applied to the walls, while the penetrations between primitives in contact are also increased. The stopping criterion is at the discretion of the user. A simple criterion would be to stop when the desired porosity is reached.

While rigid walls may be easy to implement, the resulting domains will not be periodic; a desirable trait for subsequent prediction of volume averaged properties. To obtain periodic domains, the rigid walls must be replaced with periodic boundary conditions. Periodic boundary conditions can be implemented by 'wrapping' the coordinates of all the primitives inside the domain, a concept illustrated in Fig. 1.

In Fig. 1, Primitive A is wrapped across a flat periodic interface in the x-direction to form primitive A'. A' acts as a proxy for A; the collision between A' and B is treated as a collision between A and B. In contrast to a rigid wall the periodic boundary does not apply a direct force to the primitives in contact. If the domain is