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Mesosopic modeling of the effective thermal conductivity of random open-cell porous foams

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Abstract: Although highly desirable, accurate prediction of the effective thermal conductivity of random open-cell porous foam materials has remained to be a challenging problem. Aimed at the most thorny obstacles, we have developed in this paper a random generation-growth method to reproduce the microstructures of open-cell foam materials via computer algorithm, and then solve the energy transport equations through the complex structure by using a high-efficiency lattice Boltzmann method. The effective thermal conductivities of open-cell foam materials are thus numerically calculated. The comparisons between the predictions and existing experimental data lead to the following conclusions. First the predicted thermal conductivity caused by pure thermal conduction is lower than the experimental data when the thermal conductivity is relatively low, and the radiation heat transfer is non-negligible during the thermal transport in the materials. After adjusting for radiation effect, the numerical predictions agree rather well with the experimental data for high porosity cases. However as the material porosity decreases, the radiation influence is diminishing, xxx In general the effective thermal conductivity of open-cell foam materials is much higher than that of granular materials of the same components due to the enhanced heat transfer by the inner netlike morphology of the foam materials.

Keywords: *effective thermal conductivity; open-cell foams; random structure; mesoscopic modeling; random generation growth; lattice Boltzmann method.*

1. Introduction

An ever increasing interest has been focused on heat and mass transfer processes in porous media due to their growing importance in functional material design, thermal managements of microsystems, and even in bio-medical engineering [1-5]. Among them the high-porosity foam materials are novel industrial materials with low density and unique transport properties, different from those of conventional porous media, which bring them to special and important applications [6,7]. For examples, the metal and ceramic foams have been used in design of aircraft wing structure in the aerospace industry, in catalytic surfaces for chemical reactions, as the core structure for high strength panels, and the containment matrix and burn rate enhancer for solid propellants [7,8]. More recently, the metal foams have been considered as potential candidates for heat sinks and compact heat exchangers due to their relatively high thermal transport capability yet with a low density, as opposed to the polymeric foams that have been used as the efficient thermal insulation materials because of the poor thermal transport performance [9-12]. All these applications require accurate evaluations of the effective thermal transport properties of such porous foam materials.

Several models have been proposed for modeling and predicting the effective thermal conductivity of open-cell porous foam materials, which have been summarized and reviewed in some excellent publications [7,13-15]. Dul'nev used a cubic frame to represent the open-cell structure so as to develop an analytical model [16,17]. Calmidi and Mahajan [18] presented a one-dimensional thermal conduction model by considering the porous structure as a two-dimensional array of hexagonal cells, where the contribution of lump at the intersection was taken into account by varying the shape of an artificial blob of metal at the intersection [19]. Boomsma and Poulikakos [20] proposed a one-dimensional heat conduction model based on a three-dimensional tetrakaidecahedral frame description of the structure. Another interesting geometric model is to represent the foam structure by considering a homogeneous dispersion of spherical voids in a solid matrix; several researchers have used this model for a fully numerical prediction of the effective thermal conductivities of foam materials [22,23]. Most recently Schmierer and Razani have developed a new geometric model with spherical nodes and then numerically calculated the effective thermal conductivities of open-cell porous media [21].

Given the efforts and advances on the topic, the problem is still far away from a perfect solution. First, almost all the existing models are based on idealized periodic arrays with regular geometries where the stochastic characteristics are ignored so that generally none of them work well over wide porosity range. Second, most the analytical models involve parameters whose values have to be determined empirically by *ad hoc* experiments. Third, for the existing numerical models, both the geometry complexity and the conjugate heat transfer boundary conditions in case of such porous media require extremely fine grid, often causing prohibitively high computation cost and thus limiting the computed domain into a small special region.

In this contribution, we introduce a random generation-growth method to reproduce the microstructures of open-cell foam materials by computer algorithms as we did for granular and fibrous materials [24-26], and then to solve the energy transport equations through complex structure using a high-efficiency lattice Boltzmann method. The calculated effective thermal conductivities of the open-cell foam materials will be compared with various experimental data and other theoretical solutions, and the thermal characteristics of such materials will then be investigated.

2. Numerical methods

The numerical methods used in this work include a random generation-growth algorithm for reproducing the microstructures of open-cell foam materials and a lattice Boltzmann algorithm for solving the energy transport equations through the structures.

2.1 Random generation-growth method for netlike structures

As mentioned before, the existing models are all based on periodic arrays with regular geometries, such as hexagon and tetrakaidecahedron. In such models, the stochastic natures of the porous materials were obliterated and attentions were focused only on the shapes and contributions of the intersection nodes to the effective thermal conductivities of the systems [18-23]. Here we propose a random generation-growth method to reproduce the microstructures of open-cell foam materials with the intersection nodes forming naturally depending on the growth conditions.

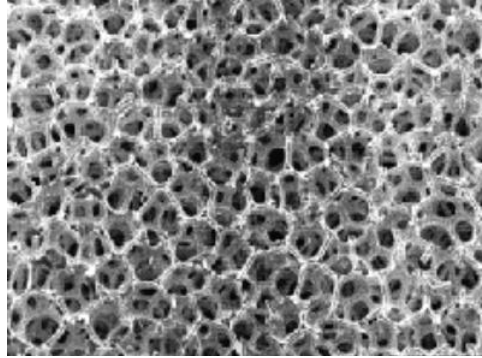


Fig. 1 Netlike microstructure of an open-cell foam material

Consider the two-phase netlike structure of an open-cell foam material shown in Fig. 1. We assume the nodes are uniformly distributed in the material. Each node is connected with N neighboring nodes by fibers (or link lines). Following the spirit of our random generation-growth methods for granular and fibrous materials, the generation process for such netlike structures is described as follows.

(1) randomly locate the nodes based on a distribution probability, c_d , which is defined as the probability of a point to become a node of the net. Each point on the grids will be assigned one random number uniformly distributed within $(0,1)$, the points whose assigned numbers are smaller than the given c_d will become the nodes of the net. The value of c_d is thus strongly related to the node number density and therefore influences the porosity of the material;

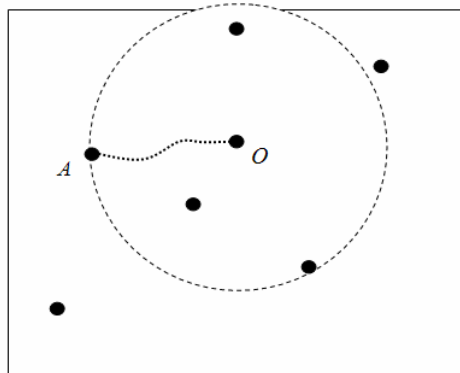


Fig. 2 Sketch illumination of searching target nodes

(2) search N target nodes to link to each of the neighboring nodes. The searching process is moving outward from an original node O as sketched in Fig. 2. We circle around the node O and each node falling into the circle will be a potential target such as the four nodes in the figure

including node A. Another random number assignment will be performed among the circled nodes and only those whose assigned random number is greater than a target probability, t_t , will be accepted as the target nodes of the original node. The target probability is set to eliminate those xx and thus is determined based on the structure expected. Repeat such searching process until each node has N target nodes respectively;

(3) grow fibers (or link lines) from each original node to its target nodes. The growths are again based on a random rule so that the links do not necessarily appear straight;

(4) widen each fiber if necessary and stop growth if the fiber diameter (d) reaches the specified value, or the porosity attains the given level ε .

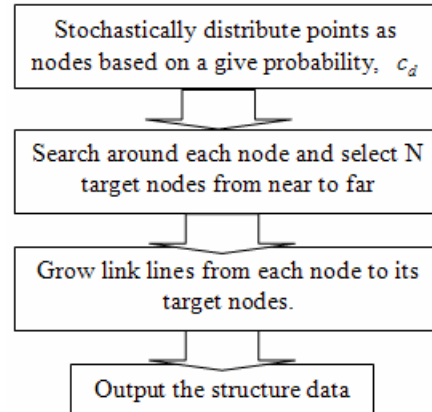


Fig. 3 Flow chart of the generation method

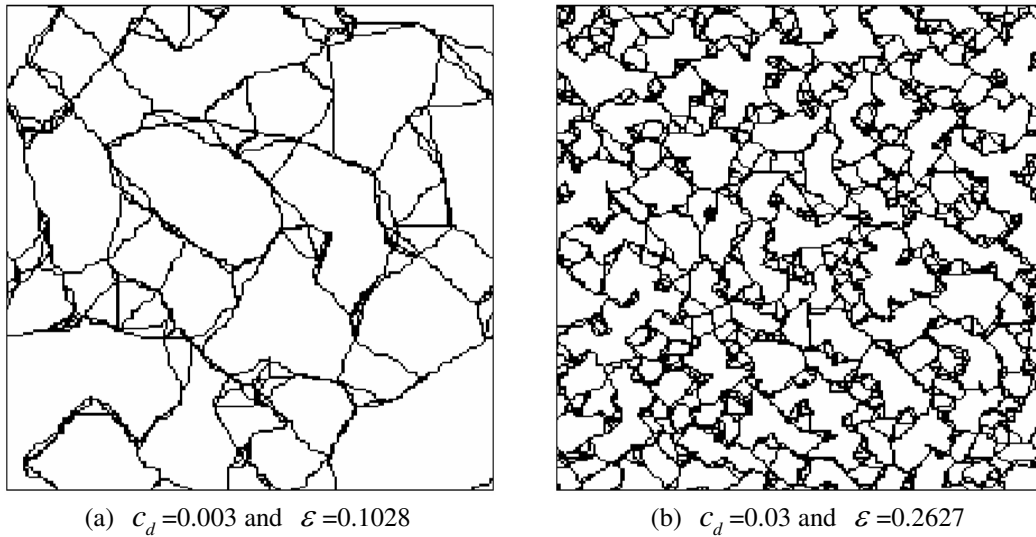


Fig. 4 Generated 2D microstructures using different parameters

The generation process can also be simply illuminated by the flow chart shown in Fig. 3. Thus the generated structures are controlled by five parameters (c_d, N, t_t, d and ε). We fixed $N=4$, $t_t=0.8$ and $d=1$ in the work of this paper and then the porosity (the volume occupied by the links) was only a result of c_d . Fig. 4 demonstrates two examples of thus generated two-dimensional microstructures on 200×200 grids. The white area represents the voids (or gas) structure and the

dark the solid link lines. The stochastic characteristics appear clearly and realistically from the structures. The intersection nodes are lean when the porosity is pretty low and grows much lump when the porosity is higher. As this random generation-growth algorithm can be readily applied to three dimensional case, we use three-dimensional structures in our simulations below.

2.2 Lattice Boltzmann method for governing equations

To calculate the effective thermal conductivity of porous materials, we have to solve the energy equations for the temperature and heat flux fields. Consider a pure thermal conduction through a porous structure with the following assumptions: two phases only; no phase change and no convection; the radiation is ignored for now. When the contact thermal resistance is negligible, the energy equations under such assumptions for thermal conduction through the two-phase porous structures without heat sources are

$$(\rho c_p)_s \left(\frac{\partial T}{\partial t} \right) = k_s \nabla^2 T \quad (1)$$

$$(\rho c_p)_v \left(\frac{\partial T}{\partial t} \right) = k_v \nabla^2 T \quad (2)$$

with the continuity constrains at the inter-phase surfaces

$$T_{s,int} = T_{v,int} \quad (3)$$

$$k_s \left. \frac{\partial T}{\partial n} \right|_{s,int} = k_v \left. \frac{\partial T}{\partial n} \right|_{v,int} \quad (4)$$

where subscript s represents the solid and v the void, and int the interfaces; T is the temperature, ρ the density, k the thermal conductivity, and c_p the specific heat capacity. Eqs (1)-(4) describe a classical case of the multiphase conjugate heat transfer problem [27]. At the two-phase interfaces, both the temperature and heat flux continuities have to be satisfied. As stated before, this interface constraint increases the computational costs tremendously when using the conventional numerical methods. Moreover, since there are huge numbers of such interfaces in many porous materials, this further pushes the computational cost into prohibition.

Recently, the lattice Boltzmann method (LBM) has been developed to solve effectively the fluid-solid conjugate heat transfer [28], which is intrinsically a mesoscopic approach based on the evolution of statistical distribution on lattices [29,30]. Due to its easy implementation of multiple interparticle interactions and complex geometry boundary conditions [31-33], the LBM has gained several successes in predicting the effective thermal conductivities of conventional porous media [24-26]. We thus propose to adopt the highly efficient LBM approach, which is also auto-conservative [24-26]. Furthermore, because of the requirement of temperature and heat flux continuities at phase interfaces, the volume thermal capacities (ρc_p) at different phases have to be maintained as the same [27]; and the conjugate heat problem between different phases can thus be solved. Here we follow our previous work using the lattice Boltzmann algorithm for the fluid-solid conjugate heat transfer problem [28].

For the pure thermal conduction in porous materials governed by Eqs. (1)-(4), the temperature evolution equation for a three-dimensional fifteen-speed (D3Q15) LBM can be generally given as [25,28],

$$g_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta_t, t + \delta_t) - g_\alpha(\mathbf{r}, t) = -\frac{1}{\tau} [g_\alpha(\mathbf{r}, t) - g_\alpha^{eq}(\mathbf{r}, t)], \quad (5)$$

where \mathbf{r} is the location vector, t the real time, δ_t the time step, g^{eq} the equilibrium

distribution of the evolution variable g_α

$$g_\alpha^{eq} = \begin{cases} 0 & \alpha = 0 \\ T/9 & \alpha = 1 \text{ to } 6 \\ T/24 & \alpha = 7 \text{ to } 14 \end{cases}, \quad (6)$$

\mathbf{e}_α is the discrete velocity

$$\mathbf{e}_\alpha = \begin{cases} (0,0,0) & \alpha = 0 \\ (\pm 1, 0, 0)c, (0, \pm 1, 0)c, (0, 0, \pm 1)c & \alpha = 1 \text{ to } 6 \\ (\pm 1, \pm 1, \pm 1)c & \alpha = 7 \text{ to } 14 \end{cases}, \quad (7)$$

and τ the dimensionless relaxation time for each phase which is determined by the thermal conductivity of each phase,

$$\tau_s = \frac{3}{2} \frac{k_s}{(\rho c_p)_s \cdot c^2 \delta_t} + 0.5, \quad (8)$$

and

$$\tau_v = \frac{3}{2} \frac{k_v}{(\rho c_p)_v \cdot c^2 \delta_t} + 0.5, \quad (9)$$

Here we have to set $(\rho c_p)_s$ equal to $(\rho c_p)_v$ in the simulations to assure the continuity at the interfaces [27]; also c is the *pseudo* sound speed, defined as δ_x / δ_t where δ_x is the lattice constant (i.e., the grid size), whose value can take any positive numbers theoretically only to insure the values of τ within (0.5, 2) [34].

The temperature and the heat flux can be then calculated respectively by [27,35]

$$T = \sum_{\alpha} g_{\alpha} \quad (10)$$

$$q = \left(\sum_{\alpha} \mathbf{e}_{\alpha} g_{\alpha} \right) \frac{\tau - 0.5}{\tau} \quad (11)$$

For the isothermal boundary treatment, we follow the bounce-back rule of the non-equilibrium distribution proposed by Zou and He [36]. For the insulated boundary, a specula reflection treatment is implemented to avoid energy leak along the surfaces [24]. After the temperature field is solved, the effective thermal conductivity, k_{eff} , can be determined:

$$k_{eff} = \frac{L \cdot \int q \cdot dA}{\Delta T \int dA} \quad (12)$$

where q is the steady heat flux through the media cross section area dA between the temperature difference ΔT with a distance L . All of these parameters can be theoretically determined, and thus there are no empirical factors existed in the model.

3. Results and discussion

Since our lattice Boltzmann solver has been validated by several theoretical solutions and experimental data for granular porous media in our previous work [24,25], we are comparing our present numerical results for open-cell foam materials with the existing experimental data directly.

In our simulations, the porous structures are generated on a $50 \times 50 \times 50$ grid, and then the energy transport governing equations solved through the structures by the high-efficiency lattice Boltzmann method. As shown in Fig. 4, our generated porous structures show remarkable stochastic features, thus leading to fluctuations around an averaged result for each trail with given parameters. We have studied such numerical uncertainty and found that the fluctuation is strongly dependent on the grid number and slightly affected by the solid volume fraction. A larger grid number and higher solid volume fraction will lead to smaller fluctuations. However for the simulations in the present work, the fluctuations are roughly smaller than 5%.

Fig. 5 shows the predicted effective thermal conductivities of reticulated vitreous carbon (RVC) foams with water or air as the fluid media, compared with the existing experimental data [19]. The component thermal conductivities used in the simulations are $k_{RVC}=8.5$ W/m K, $k_{water}=0.615$ W/m K and $k_{air}=0.026$ W/m K [14,37]. The RVC-water predictions agree well with the experimental data while the RVC-air predictions are a little lower than the experimental results. We noticed that the ambient temperature was 25 °C when performing the experimental measurements [19]. Therefore the underestimation of the effective thermal conductivity of RVC-air foams could result from the neglected thermal radiation. The effects of thermal radiation may become more significant when the overall effective thermal conductivity of media is relatively low.

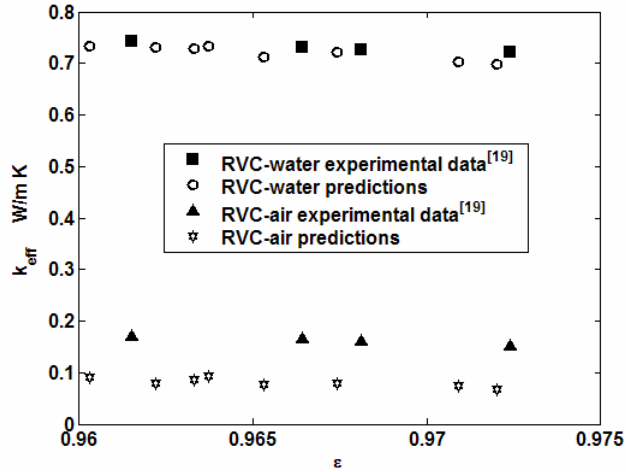


Fig. 5 Comparisons of effective thermal conductivities in RVC foams

To verify our speculation, we have added the thermal radiation contribution to our calculation using the existing models for radiative heat transfer. Tao et al. [12] have proposed a simple relationship between the radiation contribution k_{rd} to the thermal conductivity and the temperature T for polyurethane (PU) foams as:

$$k_{rd} = \frac{16\sigma T^3}{3(42.038\rho_s V_s + 121.55)} \quad (13)$$

where σ is the Stefan-Boltzmann constant (5.67×10^{-8} W/m²K⁴), T the mean temperature, ρ_s the solid density and V_s the solid volume fraction.

Fig. 6 shows the predictions of effective thermal conductivities of PU foams at 286 °K with and without the radiation modification, in comparison with experimental data [11,12]. The parameters used in the simulations are the thermal conductivity of PU solid $k_{PU}=0.262$ W/m K, the thermal conductivity of air at 286 °K and under a standard pressure $k_{air,sp}=0.0252$ W/m K [37], the thermal

conductivity of air at 286 °K and under a low pressure (nearly 2 Pa) $k_{air,lp} = 5 \times 10^{-7}$ W/m K, and the PU solid density $\rho_s \approx 800$ kg/m³ [6]. After the radiation modification the effective thermal conductivities agree pretty well with the experimental data for PU foams under both a standard air pressure and a low air pressure as seen in Fig. 6. The results also show that the importance of radiation contribution decreases with an increasing solid volume fraction so that the two simulation results converge at high solid volume fraction; e.g., the radiation contribution accounts for almost 6% when the solid volume fraction is over 10% for 286 °K and standard air pressure conditions, as indicated in Fig.6.

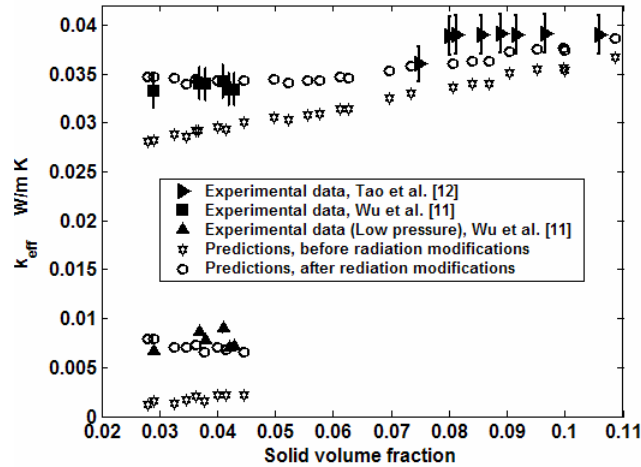


Fig. 6 Comparisons of effective thermal conductivities against the solid volume fraction in polyurethane foams. The solid symbols are experimental data, the stars are predicted results before radiation modifications and the circles are predictions after modifications.

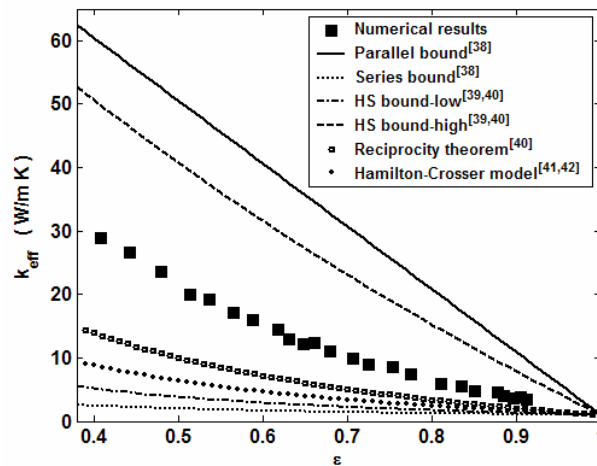


Fig. 7 Comparisons of effective thermal conductivity versus the porosity in open-cell foams with $k_s = 100$ W/m K, and $k_v = 1$ W/m K.

After comparisons with experimental data, our numerical results have also been compared with predictions from some theoretical and empirical models in Fig. 7. The component thermal properties are chosen as $k_s = 100$ W/m K, and $k_v = 1$ W/m K, and the porosity varies from 0.4 to 0.92. The solid line and the dotted line are classical bounds of parallel and series models

respectively [38]. The dash-dot line and the dashed line are the lower and upper bounds by Hashin and Shtrikman (HS) respectively [39,40]. The Maxwell model for spherical particle porous media gives the same predictions as the HS lower bounds [38]. The open circles are based on the reciprocity theorem [40], whose predictions agreed well with many granular materials. The solid circles are from the Hamilton-Crosser model for cylindrical particle porous media [41,42]. The comparisons indicate that the effective thermal conductivity of open-cell porous media is much higher than those of the granular porous media, i.e., the netlike microstructure enhances the thermal conduction in open-cell form materials. However the effective thermal conductivities are still within the lower and upper bounds of the Hashin and Shtrikman model.

4. Conclusions

A random generation-growth method has been developed to reproduce much more realistic microstructures of open-cell foam materials by computer algorithms. The energy transport equations through the complex structure are then solved using a high-efficiency lattice Boltzmann method. The effective thermal conductivities of open-cell foam materials are thus derived. The comparisons between the predictions and existing experimental data show that the radiation heat transfer is a non-negligible factor for thermal transports in high-porosity low-conductivity open-cell foam materials at low porosity range. After radiation modification, the numerical predictions of effective thermal conductivities agree well with the experimental data. The importance of the radiation contribution decreases however when the solid volume fraction increases. The effective thermal conductivity of open-cell foam materials is much higher than that of granular materials with the same components and at the same porosity. In other words, the inner netlike morphology of such foam materials actually enhances the heat transfer capacity of the materials.

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