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Numerical Predictions of the Effective Thermal Conductivity of the Rigid Polyurethane Foam

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Abstract: A reconstruction method is proposed for the polyurethane foam and then a complete numerical method is developed to predict the effective thermal conductivity of the polyurethane foam. The finite volume method is applied to solve the 2D heterogeneous pure conduction. The lattice Boltzmann method is adopted to solve the 1D homogenous radiative transfer equation rather than Rosseland approximation equation. The lattice Boltzmann method is then adopted to solve 1D homogeneous conduction-radiation energy transport equation considering the combined effect of conduction and radiation. To validate the accuracy of the present method, the hot disk method is adopted to measure the effective thermal conductivity of the polyurethane foams at different temperature. The numerical results agree well with the experimental data. Then, the influences of temperature, porosity and cell size on the effective thermal conductivity of the polyurethane foam are investigated. The results show that the effective thermal conductivity of the polyurethane foams increases with temperature; and the effective thermal conductivity of the polyurethane foams decreases with increasing porosity while increases with the cell size.

Key words: polyurethane foam; effective thermal conductivity; lattice Boltzmann method; radiation; hot disk

1 Introduction

The rigid polyurethane foam is an excellent insulation material, and has been widely used in daily life and engineering applications due to its extremely low effective thermal conductivity. Originally, CFC-11 was used as the blowing agent because of its low thermal conductivity. However, CFC-11 is not an environmentally friendly blow agent. Therefore, it was replaced by HCFC-141b and after that by cyclopentane[1,2]. Nowadays, most of the polyurethane foams in the market are still blown up by cyclopentane, and they have been the focus of the studies.

The effective thermal conductivity is an important parameter for insulation materials. The rigid polyurethane foam is the porous material with rather complicated microstructure, resulting in the difficulty in determining the effective thermal conductivity. Much attention has been devoted to the prediction of the effective thermal conductivity of the rigid polyurethane foams. Jarfelt *et al*[3] and Kuhn *et al*[4] predicted the effective thermal conductivity of the polyurethane foam resistance network model to obtain the effective thermal conductivity of the rigid polyurethane foam. Although the above theoretical methods are simple and effective, they all neglected the effect of the complicated microstructure on the effective thermal conductivities of the polyurethane foams. As for the numerical method, Ma *et al*[6] used the finite element method to calculate the thermal conductivity of carbon foams for the complete range of porosity. Wang *et al*[7] applied the lattice Boltzmann method (LBM) to obtain the effective thermal conductivity of the polyurethane foam based on the digitalized scanning electron microscope (SEM) picture but neglecting the influence of radiation on the effective thermal conductivity. Dohrn *et al*[8] adopted the transient hot wire method and Wu *et al*[9] used the measurment system made by the EKO to determine the effective thermal conductivity of polyurethane foams.

Radiation is an important contribution part to the

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effective thermal conductivity of polyurethane foams. Although much research has considered the influence of the radiation on the effective thermal conductivity of the polyurethane foams, they simply assume that the polyurethane foams are optical thickness materials and then solved the Rosseland approximation equation rather than the radiative transfer equation to obtain the radiative thermal conductivity[3,4]. Mendes *et al*[10] pointed out that the Rosseland approximation equation can only be applied to the optical thickness larger than 10.

In the present paper, the combination of finite volume method (FVM) and lattice Boltzmann method (LBM) is adopted to numerically predict the effective thermal conductivity of polyurethane foams. First, FVM is applied to obtain the conductive thermal conductivity, λ_c, of the 2D heterogeneous polyurethane foams. Then, we treat it as a 1D homogeneous material with the determined conductive thermal conductivity. Meanwhile, The LBM is applied to solve the 1D radiative transfer equation, and further to obtain the radiative heat flux and its divergence. Finally, the LBM is used to solve the 1D conduction-radiation energy transport equation to obtain the effective thermal conductivity of the polyurethane foams considering the combined effect of conduction and radiation. To validate the accuracy of the present method, the hot disk method is used to measure the effective thermal conductivity of the polyurethane foams at different temperature. After validation, a reconstruction method for polyurethane foams is proposed to investigate the effect of the porosity and cell size on the effective thermal conductivity of the polyurethane foams.

2 Numerical method

In the present paper, we solve the 1D conduction-radiation energy transport equation considering the combined effect of conduction and radiation:

$$\frac{\partial T}{\partial t}=\left(\frac{\lambda_{\text{eff,c}}}{\rho c_{\text{p}}}\right)\frac{\partial^2 T}{\partial^2 x}-\frac{1}{(\rho c_{\text{p}})}\frac{\partial \bar{q}_{\text{r}}}{\partial x} \tag{1}$$

where $\lambda_{\text{eff,c}}$ is the conductive thermal conductivity of the 2D heterogeneous conduction, and $\partial \bar{q}_{\text{r}}/\partial x$ is obtained by solving the 1D radiative transfer equation. The total effective thermal conductivity of the polyurethane foams can be obtained by

$$\lambda_{\text{e}}=\frac{(q_{\text{c}}+q_{\text{r}})}{\Delta T/L} \tag{2}$$

2.1 LBM for conduction-radiation energy transport equation

A D1Q2 LB model is adopted to solve the 1D conduction-radiation energy transport equation (Eq. (1)). The evolution equation for the temperature distribution function is shown below[11,12].

$$f_i(\bar{r}+\bar{e}_i\Delta t,t+\Delta t)=f_i(\bar{r},t)-\frac{\Delta t}{\tau}[f_i(\bar{r},t)-f_i^{\text{eq}}(\bar{r},t)]-\frac{\Delta t}{\rho c_{\text{p}}}w_i\frac{\partial \bar{q}_{\text{r}}}{\partial x} \tag{3}$$

where $\bar{r}$ denotes the particle position; t is the real time; Δt is the time step; f_i is the temperature distribution function; f_i^{eq} is the equivalent temperature distribution function, and is defined as (D1Q2 model):

$$f_i^{\text{eq}}=w_iT,\quad i=1, 2 \tag{4}$$

where w_i=1/2. The relation between the relaxation time coefficient τ and the conductive thermal conductivity $\lambda_{\text{eff,c}}$ is[11]

$$\tau=\frac{\lambda_{\text{eff,c}}}{(\rho c_{\text{p}})}\frac{1}{c^2\Delta t}+0.5 \tag{5}$$

where c is the lattice speed.

The local macroscopic temperature can be obtained by the summation of the discrete temperature distribution functions:

$$T=\sum_{i=1}^{2}f_i \tag{6}$$

The local conductive heat flux can be obtained by[13]:

$$q_{\text{c}}=-\rho c_{\text{p}}(f_1-f_2)c\frac{\tau-0.5}{\tau} \tag{7}$$

2.2 FVM for 2D heterogeneous conduction

Considering a 2D steady heat conduction process without any heat source term, the energy conservation equation is:

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)=0 \tag{8}$$

Integrating Eq.(8) over the control volume P (shown in Fig.1), we can obtain the discretization equation of the energy governing equation[14]:

$$\begin{cases}a_{\text{P}}T_{\text{P}}=a_{\text{E}}T_{\text{E}}+a_{\text{W}}T_{\text{W}}+a_{\text{N}}T_{\text{N}}+a_{\text{S}}T_{\text{S}}\\ a_{\text{P}}=a_{\text{E}}+a_{\text{W}}+a_{\text{N}}+a_{\text{S}}\\ a_{\text{E}}=\lambda_{\text{e}}\Delta y/\delta x_{\text{e}},\ a_{\text{W}}=\lambda_{\text{w}}\Delta y/\delta x_{\text{w}},\\ a_{\text{N}}=\Delta x/\delta y_n, a_S=\lambda_{\text{s}}\Delta x/\delta y_{\text{s}}\end{cases} \tag{9}$$

In this case, each control volume is occupied by the gas or solid (polyurethane resin) phase. The hamonic mean method is adopted to determine the thermal conductivity at the interface[14]:

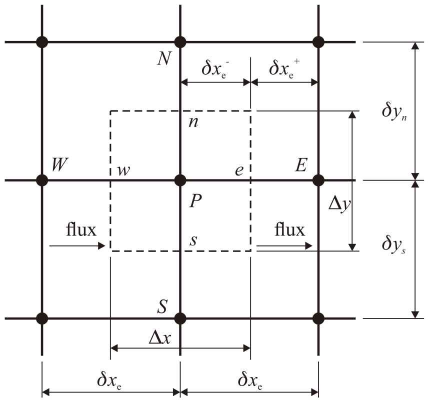


Fig.1 Grid system in Cartesian coordinates

$$\frac{(\delta x)_e}{\lambda_e}=\frac{(\delta x)_e^-}{\lambda_P}+\frac{(\delta x)_e^+}{\lambda_E} \tag{10}$$

For the computational domain, the right and left boundaries are set to be isothermal but at different temperature, while the top and bottom boundaries are set to be adiabatic. If the temperature field is converged, the conductive thermal conductivity of the polyurethane foam can be obtained by:

$$\lambda_c=\frac{\int q_c \mathrm{d}A}{\Delta AT/L} \tag{11}$$

2.3 LBM for radiative transfer equation

After obtaining the conductive thermal conductivity of the 2D heterogeneous material, we treat it as a 1D homogenous material with the given equivalent thermal conductivity, and then solve the 1D conduction-radiation energy transport equation to obtain the combined conduction-radiation effective thermal conductivity. We assume that the radiation transfers only along the x direction by neglecting the temperature difference in y direction because other boundaries are assigned to be adiabatic. To solve the conduction-radiation energy transport equation, we should first determine the divergence of radiative heat transfer. Here, we adopt the LBM to solve the 1D radiative transfer equation to obtain $\partial \vec{q}_r/\partial x$.

For the absorbing, emitting and scattering medium, the radiative transfer equation in any direction s can be described as[15]:

$$\frac{\mathrm{d}I(\vec{r},\vec{s})}{ds}=-\beta I(\vec{r},\vec{s})+\beta S \tag{12}$$

where I is the intensity, β is the extinction coefficient, and S is the source term given by[15]:

$$S=(1-\omega)I_b(\vec{r})+\frac{\omega}{4\pi}\int_{\Omega'=4\pi} I(\vec{r},\vec{s})\Phi(\vec{r},\vec{s}',\vec{s})\mathrm{d}\Omega' \tag{13}$$

where ω is the scattering albedo, $\Phi(\vec{r},\vec{s}',\vec{s})$ is the scattering phase function.

If the scattering is assumed to be isotropic, $\Phi(\vec{r},\vec{s}',\vec{s})=1$. The source term becomes:

$$\begin{aligned}S&=(1-\omega)I_b(\vec{r})+\frac{\omega}{4\pi}\int_{\Omega'=4\pi} I(\vec{r},\vec{s})\mathrm{d}\Omega'\\&=(1-\omega)I_b(\vec{r})+\frac{\omega}{4\pi}G\end{aligned} \tag{14}$$

where G is the incident radiation. We adopt D1Q8 LB model to solve Eq.(12)[11,16]:

$$\begin{aligned}I_i(\vec{r}_n+\vec{e}_i\Delta t,t+\Delta t)-I_i(\vec{r}_n,t)&=\Delta t e_i\beta(S''-I_i(\vec{r}_n,t))\\&=\frac{\Delta t}{\tau_i}(I_i^{eq}(\vec{r}_n,t)-I_i(\vec{r}_n,t))\quad i=1,8\end{aligned} \tag{15}$$

where

$$\tau_i=\frac{1}{e_i\beta},\ e_i=\frac{\Delta x}{\Delta t\cos\gamma_i},\ I_i^{eq}=S'' \tag{16}$$

For the diffuse-gray boundary condition, the unknown boundary intensities can be obtained by[11]:

$$I_i=\frac{\varepsilon\sigma T_b^4}{\pi}+\left(\frac{1-\varepsilon}{\pi}\right)2\pi\sum_{i=1}^{M/2} I_i\cos\gamma_i\sin\gamma_i\sin(\Delta\gamma_i) \tag{17}$$

Once the radiation intensities are obtained, the radiative heat flux and its divergence can be calculated by[11,16]:

$$q_r\approx 2\pi\sum_{i=1}^{M} I_i\cos\gamma_i\sin\gamma_i\sin(\Delta\gamma_i) \tag{18}$$

$$\nabla\cdot\vec{q}_r=\beta(1-\omega)(4\sigma T^4-G) \tag{19}$$

where β is the extinction coefficient, G is the incident radiation, and it can be obtained by[11,16]:

$$G\approx 4\pi\sum_{i=1}^{M} I_i\cos\gamma_i\sin(\Delta\gamma_i/2) \tag{20}$$

3 Application for polyurethane foams

3.1 Thermal conductivity of the components

To determine the effective thermal conductivity of the polyurethane foams, we should first determine the thermal conductivity of each component in polyurethane foams.

The thermal conductivity of the polyurethane resin varying with the temperature can be expressed as[17]:

$$\lambda_{bulk}=0.197\times(1+0.001\,7T) \tag{21}$$

As for the gas mixture in the closed cell of the polyurethane, its thermal conductivity can be calculated by the Wassiljewa mixing rule[18]:

$$\lambda_m=\sum_{i=1}^{n}\frac{y_i\lambda_i}{\sum_{j=1}^{n} y_j A_{ij}} \tag{22}$$

where y_i is the volume fraction of the *i*th gas, and λ_i is the thermal conductivity of the *i*th gas. In the present paper, the blowing agent of the polyurethane foam is the cyclopentane.

3.2 Extinction coefficient

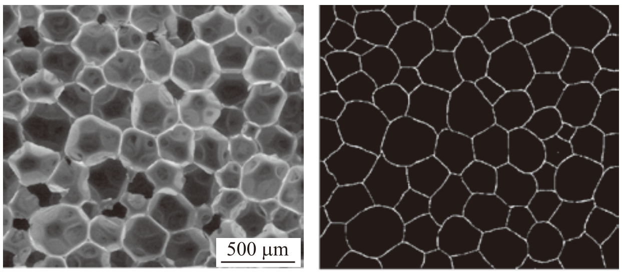
The extinction coefficient of the polyurethane foams should be determined to solve the 1D radiative transfer equation. The extinction coefficient of the polyurethane foams can be obtained by [3]:

$$\beta = 4.10\frac{\sqrt{\dfrac{f_s\rho_f}{\rho_s}}}{d} + \left[\frac{(1-f_s)\rho_f}{\rho_s}\right]\beta_w \tag{23}$$

where d is the cell diameter; ρ_f is the density of the polyurethane foam; ρ_s is the bulk density of the polyurethane resin; f_s is the volume fraction of the solid in struts; β_w is the extinction coefficient of the cell wall, and β_w=60 000 m^{-1}.

3.3 Microstructure

The effective thermal conductivity of the polyurethane foam depends on its microstructure. The scanning electron microscopic (SEM) image of the polyurethane foam and its digitalization are shown in Fig.2.



(a) SEM (b) Digitalized microstructure

Fig.2 SEM of polyurethane foam (a) and its digitalization (b)

Based on the digitalized structure of the polyurethane foams, we can numerically predict its effective thermal conductivity using the present method. Meanwhile, the hot disk method is adopted to measure the effective thermal conductivity of the sample to validate the accuracy of the present method. Although the SEM image of the polyurethane foam is an intuitive method to obtain the microstructure of the material, it costs too much resource if lots of samples need to be determined. To investigate the influence of the porosity and cell size on the effective thermal conductivity of the polyurethane foams, a reconstruction method for regenerating the microstructure of the polyurethane foams is needed. Wang *et al*[19] proposed a QSGS method for granular materials and developed a random generation growth method for the open-cell porous material[7], but they are not suitable for reconstructing the microstructure of the closed-cell polyurethane foams. In the present paper, we propose a simple but effective method to reconstruct the microstructure of the polyurethane foams.

(1) Locate a random point at the computational domain as the center of the circle;

(2) Generate a circle with a random diameter selected within a certain range to represent the closed cell, and select a random number as the thickness of the outer edge of the circle within a reasonable range to represent the solid wall of the polyurethane foam;

(3) Restrict the position of the center of a circle to be generated, making its distance from other centers of the generated circles within a reasonable range to ensure the solid wall continuous;

(4) Repeat step (3) until the porosity of the computational domain reaches the given value.

3.4 Experimental measurement

In the present paper, the hot disk method[20-22] is used to measure the effective thermal conductivity of the polyurethane foam. The experimental system contains hot disk thermal constant analyser (type: TPS2500S), temperature control system, environmental chamber and so on.

During the measurement, the hot disk probe operates as the heat source as well as the temperature sensor. The hot disk probe should be placed between two identical specimen halves. A heat pulse is then supplied by the probe to generate a dynamic temperature field within the specimens. The temperature increment of the hot disk probe surface facing the specimens depends on the thermal properties of the specimens, and it can be expressed as[20]:

$$\Delta T(\tau) = \frac{P_0}{\pi^{3/2} r\lambda} D(\tau) \tag{24}$$

After dealing with the recorded temperature increase curve, one can determine the thermal conductivity and thermal diffusivity of the specimen simultaneously.

4 Results and discussion

In the present paper, we solve the 1D homogeneous conduction-radiation energy transport equation to obtain the effective thermal conductivity of the polyurethane foams considering the combined effect of conduction and radiation. To solve Eq.(1), we need some input parameters, such as the conductive thermal conductivity of 2D heterogeneous conduction $\lambda_{\text{eff,c}}$ and the divergence of radiative heat flux $\nabla\cdot\vec{q}_r$. FVM is applied to obtain the conductive thermal conductivity of 2D heterogeneous conduction $\lambda_{eff,c}$, and LBM is adopted to solve the 1D radiative transfer equation to obtain the $\nabla\cdot\overline{q}_r$.

4.1 Comparisons of the numerical results and experimental data

In the present paper, numerical predictions of the total effective thermal conductivity of the polyurethane foam based on SEM shown in Fig.2 are compared with the experimental data measured by hot disk method. Fig.3 shows the comparison of the effective thermal conductivity of the polyurethane foam between the numerical results and experimental data at different temperature. It can be seen that the numerical results agree well with the experimental data. The maximum deviation is within ±4.5%. The effective thermal conductivity of the polyurethane foams increases with the temperature. It is because both the thermal conductivities of the solid wall (polyurethane resin) and gas mixture increase with the temperature.

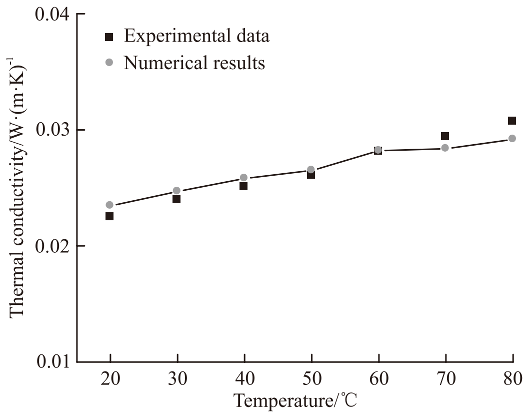
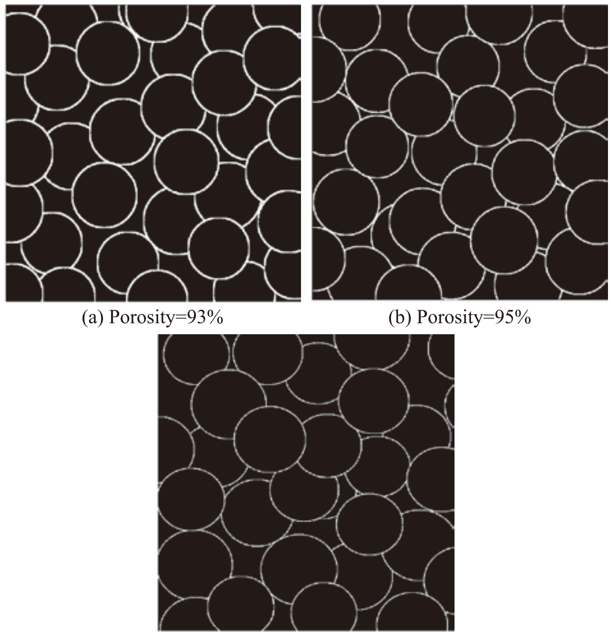


Fig.3 Comparisons of the numerical results and experimental data

4.2 Effect of porosity

To investigate the effect of the porosity on the effective thermal conductivity of the polyurethane foams, lots of microstructures with different porosities should be reconstructed first. Figs.4(a), (b) and (c) show the reconstructed microstructures of the polyurethane foam with porosity of 93%, 95%, and 97%, respectively.

Based on the reconstructed microstructures of the polyurethane foams, we applied the present method to numerically predict their effective thermal conductivities. The variation of the effective thermal conductivity of the polyurethane foams with the porosity is shown in Fig.5. It can be seen that the effective thermal conductivity of the polyurethane foams rapidly decreases with increasing porosity. It is because the thermal conductivity of the polyurethane resin is much higher than that of the cell gas mixture in polyurethane foams. The proportion of the polyurethane resin decreases with increasing porosity, resulting in the decreasing effective thermal conductivity of the polyurethane foams.



(a) Porosity=93% (b) Porosity=95%

(c) Porosity=97%

Fig.4 Reconstructed microstructures with different porosity

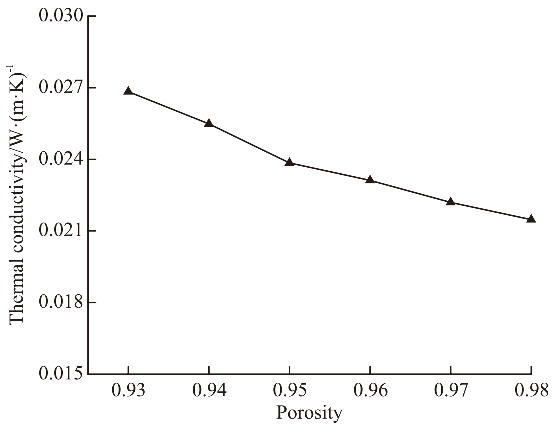
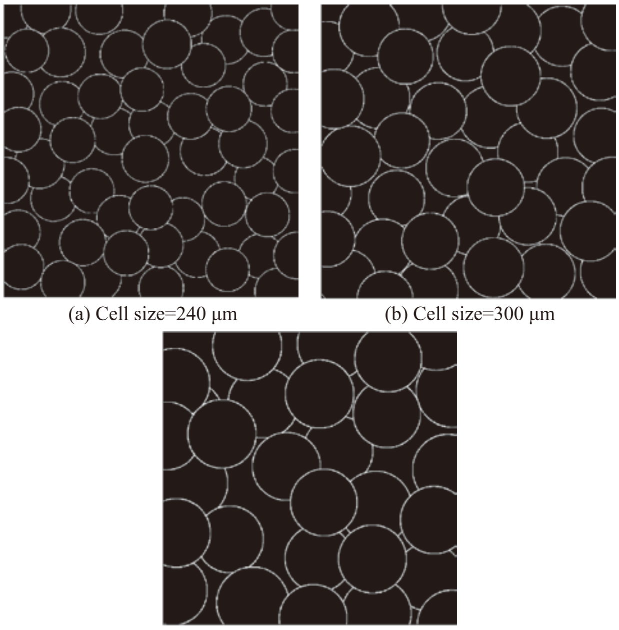


Fig.5 Effective thermal conductivity varied with the porosity

4.3 Effect of the cell size

To investigate the effect of the cell size on the effective thermal conductivity of the polyurethane foams, lots of microstructures with different cell sizes should be reconstructed first. Figs.6(a), (b) and (c) show the reconstructed microstructures of the polyurethane foam with the cell size of 240, 300, and 360 μm, respectively. Based on the reconstructed microstructure, we numerically predict the effective thermal conductivities of the polyurethane foams. The variation of the effective thermal conductivity of the polyurethane foams with the cell size is shown in Fig.7. It can be seen that the effective thermal conductivity of the polyurethane foam increases with the cell size. The reason can be attributed to the increasing conductive and radiative thermal conductivities with the cell size. The conductive thermal conductivity of 2D heterogeneous polyurethane foams can be obtained by FVM introduced in Section 2.2. As shown in Fig.7, the conductive thermal conductivity of the heterogeneous materials increases with the cell size. Furthermore, from Eq.(23), we can find that the extinction coefficient of the polyurethane foams decreases with increasing cell size, resulting in the increasing radiative thermal conductivity with the cell size.



(a) Cell size=240 μm (b) Cell size=300 μm

(c) Cell size=360 μm

Fig.6 Reconstructed microstructures with different porosity

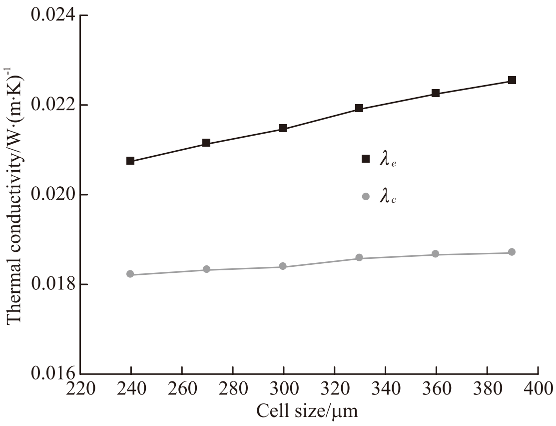


Fig.7 Effective thermal conductivity varied with the cell size

5 Conclusions

In the present paper, a reconstruction method is proposed to reconstruct the microstructure of the polyurethane foams. LBM combined with FVM is developed to numerically predict the effective thermal conductivity of the polyurethane foam. FVM is applied to solve the 2D heterogeneous pure conduction, while LBM is used to solve the radiative transfer equation and conduction-radiation energy transport equation. To validate the accuracy of the present method, hot disk method is adopted to measure the effective thermal conductivity of the polyurethane foams. We conclude that:

a) Numerical predictions of the effective thermal conductivity of the polyurethane foams agree well with the experimental data at different temperature; The effective thermal conductivity of the polyurethane foams increases with the temperature;

b) The effective thermal conductivity of the polyurethane foams decreases with increasing porosity while increases with the cell size of the polyurethane foams.

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