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Unit cells for thermal analyses of syntactic foams with imperfect interfaces

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ABSTRACT

Since there is a lack of modeling the effect of interfaces between hollow particles and matrix on the effective thermal conductivity of syntactic foams, a unit cell for the thermal analyses of syntactic foams in the presence of imperfect interfaces has been established. The model was validated with experimental data from literatures. The simulation results agree well with the experimental data. Based on the unit cell model, a parametric study was conducted to investigate the effect of interfacial thermal conductance, wall thickness and volume fraction of hollow particles on the thermal conductivity of syntactic foams. The results show that the thermal conductivity of syntactic foams increases with the increase of interfacial thermal conductance, wall thickness of hollow particles. However, the effect of volume fraction of hollow particles on the thermal conductivity of syntactic foams shows complicated dependence on the interfacial thermal conductance and wall thickness of hollow particles.

1. Introduction

Syntactic foams are hollow particle filled composites which have many unique characteristics, such as low density, low moisture absorption, high damage tolerant, low thermal conductivity and low dielectric constant [1]. Due to these characteristics, syntactic foams are widely used in many applications including marine, aeronautic and building structures. As applications of syntactic foams increase, understanding of their properties is highly required. As reported in reference [2], use of syntactic foams as thermal insulation materials is now increasing in oil and gas industry considering its low thermal conductivity. The thermal properties of syntactic foams have drawn more and more attentions in recent years. Intensive investigations [3–17] have been carried out on the theoretical and experimental aspect of thermal conductivity and coefficient of thermal expansion of syntactic foams. Recently, Zhu et al. [9] modified the surface of two kinds of Hollow Glass Microsphere (HGM) - S38HS and S60HS, which are trade names of 3 M company, with a silane coupling agent (KH570) and prepared four kinds of HGM filled low-density polyethylene(LDPE) composites-modified S38HS/LDPE composites, unmodified S38HS/LDPE composites, modified S60HS/LDPE composites and unmodified S60HS/LDPE composites. The experimental data shows that thermal conductivities increase after surface modification for S38HS/LDPE composites and S60HS/LDPE composites. This shows the importance of the interface properties between the hollow particle and the matrix on the thermal conductivity of syntactic foams. There were five existed theoretical models as discussed in the most recent publication [13], which were referred as Liang model [10–12], Felske model [14], Pal model [15], Porfiri model [16] and Park model [17]. All of these models could provide a reasonable prediction on the thermal conductivity of syntactic foams in some extent. Liang model, Felske model and Porfiri model present a simple form, however they deviate from the experimental results at high volume fraction due to their limitation. Pal model provides two important features: high volume fraction and polydispersivity. However, this model presents an implicit form and it should be solved numerically. All of these models did not account for the effect of interfacial properties on the thermal conductivity of syntactic foams.

In this paper, a three-phase rhombic dodecahedron unit cell model with imperfect interfaces was developed on the base of the unit cell approach for solid particle reinforced composites [18–20]. The model was validated with experimental results from reference [9]. The effect of interfacial thermal conductance, thermal conductivity of hollow particles, wall thickness and volume fraction on the thermal conductivity of syntactic foams were studied using this model.

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2. Modeling

The unit cell approach for solid particle reinforced composites was systematically demonstrated in references [18–20]. The unit cell was developed for the purpose of micromechanical analyses of solid particle reinforced composites with perfect interfaces at first [18]. After capability extension, it is applicable to the thermal analyses of solid particle reinforce composites [19,20]. To account for the gas inside the hollow particles and the imperfect interfaces, it should be further modified and idealized as follows:

(a) The hollow particle is modeled as a spherical shell and a spherical core. The contact between spherical and matrix is modeled.
(b) The face centered cubic packing system of the hollow particles will be used as recommended in reference [18].
(c) The effect of polydispersivity of the hollow particles was ignored because of the limitation of the unit cell approach used in this paper. However, it will not affect the following results so much, as the polydispesivity could be neglected if the polydispersivity of the hollow particles is low. In this paper, the data of S38HS and S60HS with a low dispersivity are used for model validation. In the case of high polydispersivity of hollow particles, unit cells with several hollow particles should be established to account for the factor, which could be considered in further study.
(d) The convection effects within hollow particles are negligible because of their small size and low porosity [21].

In the unit cell approach, applying the periodic boundary conditions is one of the most important steps. The relationship between macroscopic temperature gradients and the relative temperatures of two arbitrary nodes could be expressed with the following constraint equation as indicated in reference [19].

$$T' - T = (x' - x)\nabla T_x^0 + (y' - y)\nabla T_y^0 + (z' - z)\nabla T_z^0 \tag{1}$$

Where

∇T_x^0 ∇T_y^0 and ∇T_z^0 are the macroscopic temperature gradients in three directions,

T and T' are the microscopic temperature of original nodes and image nodes,

(x, y, z) and (x', y', z') are the coordinate of original nodes and image nodes.

The boundary conditions for the unit cell can be obtained by six translational transformations as shown in reference [18,19]. Under the six translational transformations, all the other cells could be fully covered by the original unit cell.

Although the constraint equations are simple, it is not easy to be implemented in ABAQUS. To implement the constraint equations into ABAQUS, all the nodes of the boundary faces should be placed carefully so that the nodes of the original face and the image face have the same relative position in their unit cells. Thus, the mesh generation method is the key to solve the problem. To ensure a uniform hexahedral mesh generation of the rhombic dodecahedron with a sphere in the center, an in-house program is developed to mesh the rhombic dodecahedron unit cell as shown in Fig. 1.

Another problem encountered in ABAQUS is that the system reports some of nodes in the boundary lines and vertices are over-constraint when the current constraint equations are used in ABAQUS directly. The source of the errors is that the nodes of boundary lines and vertices not only belong to a face. They are constrained by two or more equations. The solution to the problem is that the nodes of the boundary lines and vertices are excluded in the constraint equations. Another group of equations are established to make sure that the nodes of the boundary lines and vertices are constrained by one equation only.

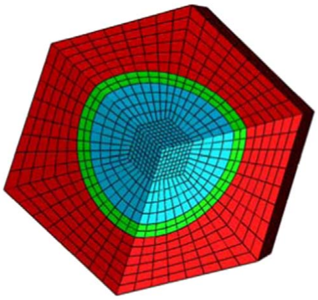

Fig. 1. Uniform hexahedral meshes of a unit cell.

3. Model validation

Experimental data from reference [9] were used to validate the proposed model. In reference [9], four kinds of HGM filled LDPE composites were prepared- modified S38HS/LDPE composites, unmodified S38HS/LDPE composites, modified S60HS/LDPE composites and unmodified S60HS/LDPE composites. The experimental data shows that thermal conductivities of the modified HGM filled composites are higher than that of unmodified HGM filled composites.

Using the proposed model, the values of thermal conductivity (k) for various values of volume fraction V_f (0–50%) and the interfacial thermal conductance h_c (0~+∞W/m^{2}K) were calculated for both modified and unmodified HGM/LDPE composites. The parameters used in the model are listed in Table 1.

As can be seen in Fig. 2(a), values of h_c 2.5×10^4 and 1.0×10^5 W/m^{2}K provided the best fit between the simulation results and the experiments data for the unmodified and modified S60HS/LDPE composites, respectively. In Fig. 2(a), the thermal conductivities of S60HS/LDPE composites with thermal insulation interfaces (h_c=0 W/m^{2}K) and perfect interfaces (h_c=+∞ W/ m^{2}K) were also calculated as the lower bound and upper bound of the model.

Theoretically, the S60HS-LDPE interfaces should be almost the same as S38HS-LDPE interfaces, because S60HS and S38HS almost have the same composition. Meanwhile, the h_c of S38HS-LDPE interfaces should have a value close to the h_c of S60HS-LDPE interfaces. Thus, the values of h_c 2.5×10^4 and 1.0×10^5 W/m^{2}K were also set in the model to calculate the thermal conductivities of unmodified and modified S38HS/LDPE composites. Then, the calculated values were compared with experimental data. As shown in Fig. 2(b), the simulation results of modified S38HS/LDPE composites agree well with the experimental values. However, the curve of unmodified S38HS/LDPE composites does not fit the experimental data exactly. It seems that the values of h_c 1.5×10^4 W/m^{2}K give the best fit of the experimental data. But it is also close to the values of h_c 2.5×10^4 W/m^{2}K.The deviation may be attributed to the large dispersion of experimental data for the unmodified S60HS/LDPE composites.

Table 1
Material properties used in the model [9].

Materials	Particle Diameter (μm)	Wall thickness (μm)	Thermal conductivity (W/mK)
HGM-S38HS	40	1.05	1.05
HGM-S60HS	30	1.29	1.05
LDPE	/	/	0.317
Gas	/	/	0.0228