

Three-dimensional numerical simulation of thermal conductivity of aluminium powder/TNT fusion-cast explosives

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Abstract: It is crucial for the preparation and performance study of fused-cast explosives to the quantitative determination of thermal conductivity, therefore, the search for a prediction method of their effective thermal conductivity has been of broad interest. The thermal conductivity of aluminium powder/TNT fused-cast explosives was investigated by numerical simulation, and a three-dimensional model of the particle-filled composite RVE was established based on DIGIMAT software, and a steady-state thermal analysis of the model was carried out using ANSYS Workbench software to investigate the impact of aluminium powder particles with different particle sizes and contents on the thermal conductivity and the effects of the mixed filler on the thermal conductivity enhancement effect of the composite when filled with the TNT matrix. The simulation results show that the theoretical thermal conductivity of Al/TNT increases exponentially with the increase of aluminium volume fraction; in the range of optimal particle size, it is more accessible to obtain composites with large thermal conductivity by filling large-size aluminium powders; in the case of low filler content, the numerical simulation results are in agreement with the results of the Maxwell-Eucken model in terms of the overall trend. The study shows that the described method can be used for predicting the thermal conductivity of Al/TNT composites.

1. Introduction

At present, the representative volume element method (RVE) has been widely used in the prediction of thermophysical properties of composites. Guo, X et al [1] designed new energy-containing conjugated polymers and calculated the thermal conductivity of the energy-containing polymers based on the Bicolano thermal conductivity calculation method and Akasaki thermal conductivity group contribution method. He, G [2] quantitatively demonstrated that pGNPs@Ag reduces the ITR, which contributes to the improving of the composite k. Lin C et al [3] doped nano-TATB particles into PBX to construct a novel self-reinforced PBX, which significantly improved the strength and toughness. Pan L et al [4] established a constitutive relationship between graphene microstructure and thermal conductivity of PBX. Pietrak, K considered the case where interfacial thermal resistance is present in the heat transfer model [5]. Burger, N examined the effect of

crystallinity, phonon scattering or filler/matrix interface on the thermal conductivity of composites [6]. The thermal conductivity of particle-filled composites has always been a hot research topic, and there are a large number of models. Still, their generality and accuracy need to be improved, and most of them contain empirical or semi-empirical parameters to be determined. The selection of research methods is mainly based on macroscopic volume-averaged or periodically distributed equivalent heat transfer units, ignoring the influence of the actual spatial structure of components on heat transfer. Although the above methods can predict for some cases, their application range is limited and cannot be applied to more situations, and their generalizability is not ideal. Thus, the study of thermal conductivity from the internal microstructure of the material is an effective way to obtain the effective thermal conductivity of composite materials.

2. Numerical simulation

2.1. RVE model

Composite materials are non-homogeneous systems, and in order to homogenize them, it is necessary to establish a reasonable analytical model and apply numerical simulation techniques to solve their microstructures. In this context, the concept of Representative Volume Element (RVE) is crucial. Table 1 shows the material parameters used to model the 3D RVE.

Table 1: Physical parameters of the materials

Materials	Thermal conductivity /W·m ⁻¹ ·K ⁻¹	Densities /g·cm ⁻³	Specific heat capacity /J·g ⁻¹ ·K ⁻¹
TNT	0.26	1.654	1.181
Al	240	1.4	0.88

2.2. Finite element model solution

The geometrical model of the microstructure can be generated by the corresponding stochastic algorithm, and then the generated stochastic geometrical model can be numerically solved by finite element. In this study, the ANSYS workbench steady-state thermal conductivity model is used to analyse the generated stochastic geometric model with finite element solution.

$$\frac{\partial}{\partial x} (k_x \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (k_y \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (k_z \frac{\partial T}{\partial z}) = 0 \quad (1)$$

Where k_x , k_y and k_z are the thermal conductivities of the material along the three main directions of the object. Since the composite material is macroscopically homogeneous, it can be viewed as consisting of an infinite number of RVE models arranged in a periodical manner, and therefore periodic boundary conditions need to be imposed on the model. The choice of boundary conditions for the RVE model has no relationship with the thermal conductivity of the composite material. Therefore, regardless of choice of boundary conditions, the value of the thermal conductivity is stabilized. Let the side length of the cubic monoclinic cell be H. The first type of boundary condition is imposed on the upper surface, i.e., the face with $y=H$ as shown in Eq. 1, and in this paper, T_{hot} is taken as 85 °C.

$$T |_{y=H} = T_{hot} \quad (2)$$

The first type of boundary condition is imposed on the lower surface, i.e., the face with $y = 0$ as shown in Eq. 2. In this paper, T_{cold} is taken as 47.5 °C.

$$T|_{y=0} = T_{cold} \quad (3)$$

The other four faces are periodic boundaries with adiabatic boundary conditions imposed as shown in Eq. (4)

$$\begin{cases} \frac{\partial T}{\partial n}|_{x=0} = 0 \\ \frac{\partial T}{\partial n}|_{x=H} = 0 \end{cases} \quad \begin{cases} \frac{\partial T}{\partial n}|_{z=0} = 0 \\ \frac{\partial T}{\partial n}|_{z=H} = 0 \end{cases} \quad (4)$$

According to the control equations and boundary conditions, the model is solved by finite elements to obtain its temperature field distribution and heat flow distribution, which combined with Fourier's steady state heat conduction law, the thermal conductivity of the composite material can be obtained. Were. Fourier's steady state heat conduction law is expressed as.

$$k = \frac{ql}{\Delta T} \quad (5)$$

where k is the thermal conductivity of the material, q is the density of heat flow through a given cross-section, l is the length in the direction of heat transfer, and ΔT is the temperature difference in the direction of heat transfer. It is usually necessary to find the average value of thermal conductivity in the three directions. This is used as the final value of thermal conductivity for this model. For ANSYS, you can use the APDL language to take out the average heat flow density along the heat flow direction on the result file, and then find out the corresponding thermal conductivity according to the corresponding thermal conductivity formula.

Figure 1 shows the finite element model of the geometric model after mesh division. The element type used in the steady-state heat conduction module of the workbench is solid186 (3D20N), where the number of mesh elements after mesh division is 461482, and the aluminium powder content is 15wt.% At that time, the number of mesh elements in the finite element model of composite materials reached 304760.

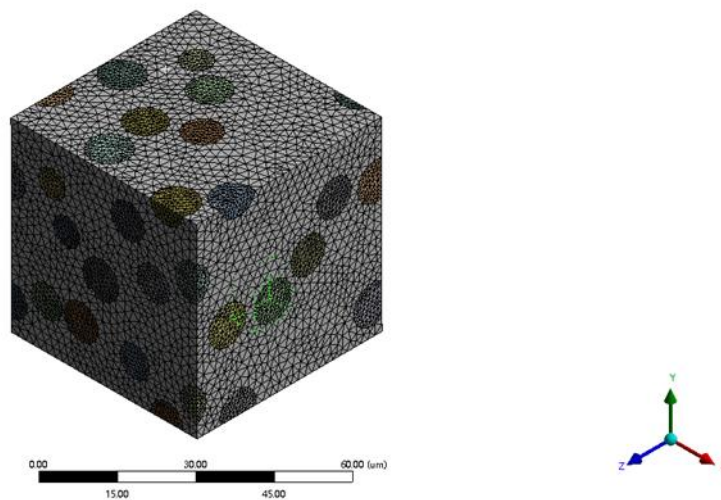


Figure 1: RVE model mesh division.

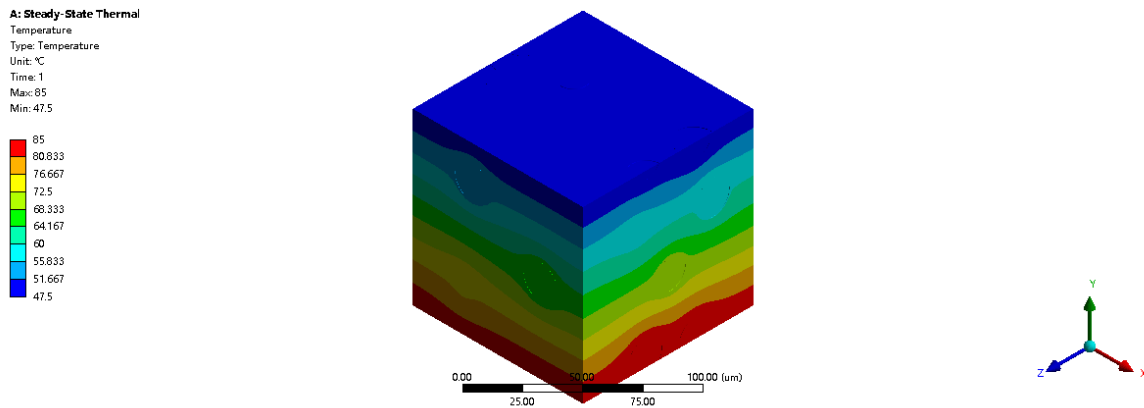


Figure 2: Temperature distribution cloud map of aluminium powder/TNT.

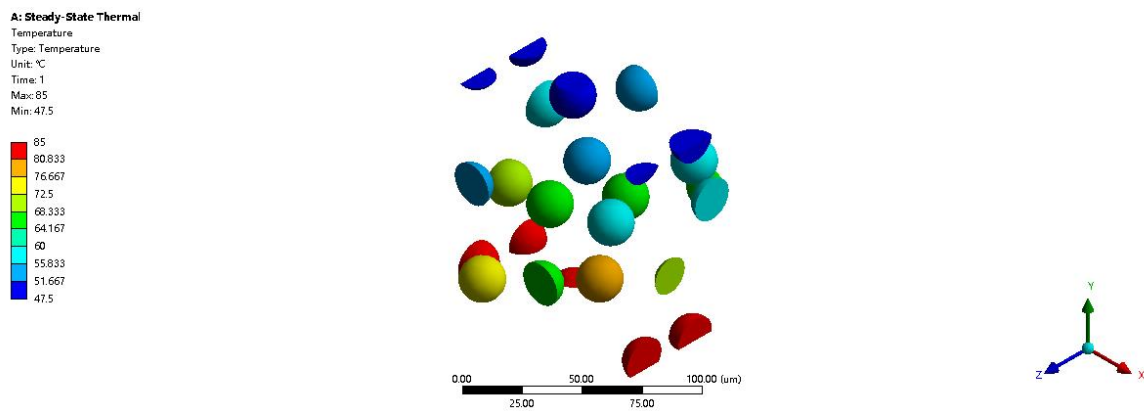


Figure 3: Thermal conductivity cloud map of aluminium powder particles.

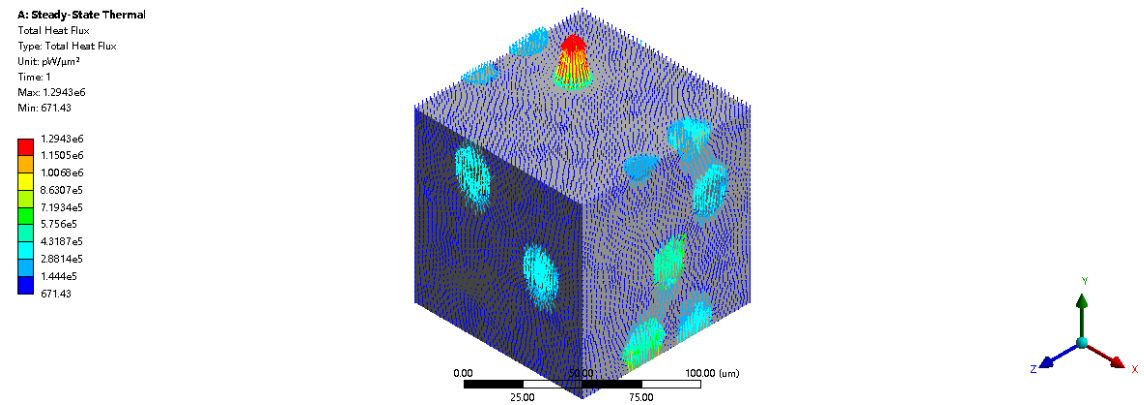


Figure 4: Heat flux vector diagram of aluminium powder/TNT.

From the temperature cloud map shown in figure 2, it can be seen that the temperature changes in each part are not the same. As shown in figure 3, the temperature gradient near the particles is smaller than that of the substrate. This is because the thermal conductivity of the filled particles is much higher than that of the substrate. According to the Fourier theorem, under the same heat flux, objects with high thermal conductivity have a smaller temperature gradient. Therefore, the temperature change near the particles is small. Figure 4 shows the heat flux vector diagram, from which it can be seen that the heat flux first aggregates from the matrix towards the particles, and then flows towards the matrix in an emitting manner.

3. Results and discussion

From the plot of the variation of theoretical thermal conductivity with the volume fraction in figure 1(a), it can be seen that the variation of the effective thermal conductivity of the TNT/Al hybrid system containing different filler volume fractions shows an exponential upward trend, which can be described by the following functional expression:

$$y = A_1 * \exp(-x/t_1) + y_0 \quad (6)$$

where A_1 , t_1 , y_0 are parameters to be determined, y is the theoretical thermal conductivity of the composite, and x is the volume fraction of aluminum powder.

Nonlinear fitting gives $A_1 = 0.38669$, $t = -0.32847$, $y_0 = -0.12965$; correlation coefficient $R^2 = 0.99738$.

3.1. Effect of the content of aluminium powder on the thermal conductivity of composites

From Figure 5(a), it can be seen that the thermal conductivity of the composite material increases with the increase of the volume fraction of filled aluminum powder, and shows an increasing trend. When the volume fraction of aluminum powder is low, the dispersion of aluminum powder particles is good, the aluminum powder particles are isolated from each other, and the interaction is weak. In the TNT/Al mixed system, an effective thermal conductivity chain cannot be formed, which hinders the enhancement of thermal conductivity by aluminum powder particles; as the filler particles of aluminum powder filler increase, cross-linking between aluminum particles gradually occurs, and thermal conductivity chains are easily formed in the TNT/Al mixed system, that is, the area with higher heat flux density in Figure 6 has higher heat flux density. Due to the significant difference in thermal conductivity between aluminum powder and TNT, the distribution of heat flux size in the model is uneven. The heat flux density inside the aluminum particles is high, with the maximum value appearing parallel to the direction of heat flux. The particles are close to the aluminum powder, while the heat density inside the TNT matrix is small. Therefore, the overall heat flux density of the TNT/Al mixed system increases with the increase of the mass fraction of aluminum particles. As a result, the thermal conductivity of the composite material was improved.

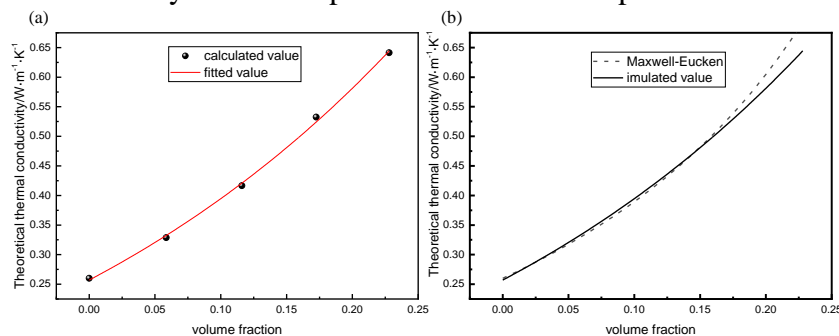


Figure 5: Variation curve of theoretical thermal conductivity of TNT/Al with volume fraction of aluminium powder.

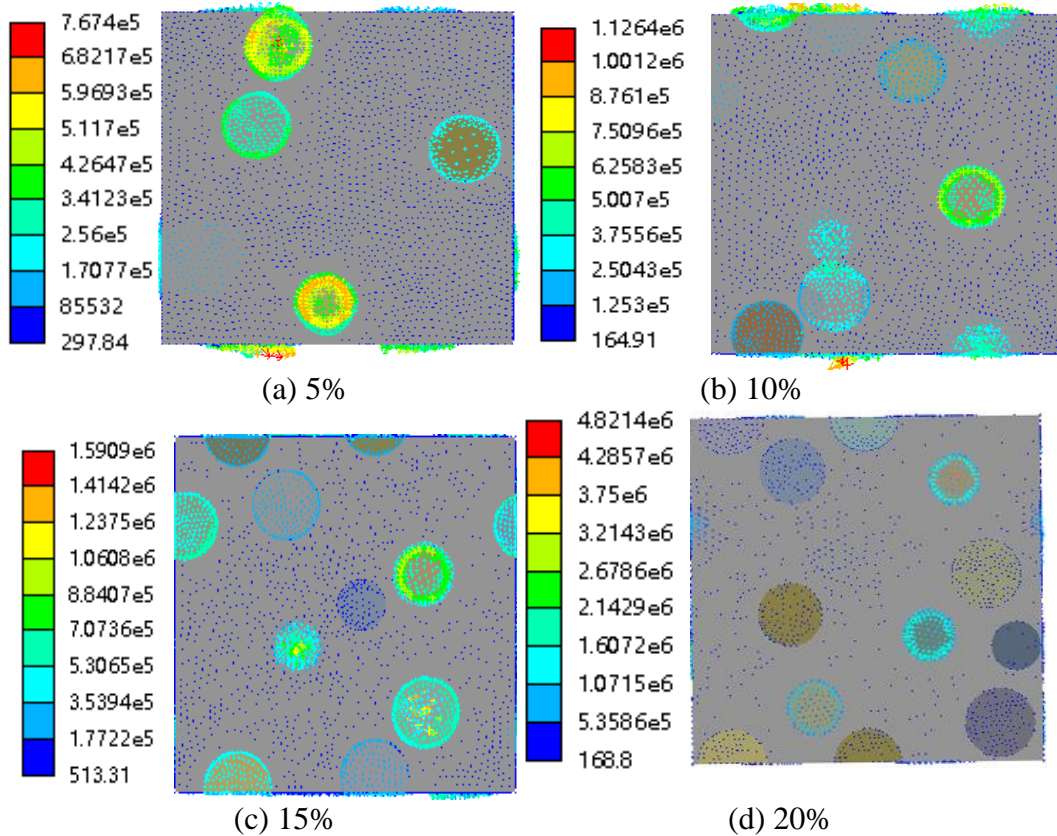


Figure 6: Heat flow vectors for different mass fractions of aluminium powder/TNT.

3.2. Effect of particle size of aluminium powder on thermal conductivity of composites

In the case of aluminium powder mass fractions of 5%, 10%, 15%, the filling simulation of different particle sizes, the results are shown in Figure 7, in the filling of the same number of parts, the optimal range of particle size under the premise of the relatively low filler (less than 10%) of the thermal conductivity of the composite material with the increase in the particle size of the aluminium powder with the tendency to increase and then reduce, because the larger the particle size of the aluminium powder means that the larger the surface area, the heat transfer path The shorter the heat transfer path. It is easier to contact each other in the TNT matrix to form a more perfect thermal conductivity chain, of course, this enhancement is not the larger the particle size of the aluminium powder the better, there is a critical diameter of aluminium powder particle size, more than the critical diameter of the thermal conductivity of the composite material is not only any enhancement, but also will destroy the integrity of the matrix, resulting in a decline in thermal conductivity. For relatively high filling amounts, the thermal conductivity of the composite material decreases with the increase of the diameter of the aluminium powder. For the aluminium powder with a particle size of 1 micron, due to the small particle size effect, the specific surface area is larger, the opportunity to contact with the surrounding medium increases, and more thermal conductivity network is formed, thus the thermal conductivity of the composite material is enhanced.

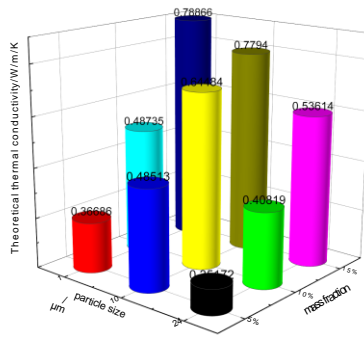


Figure 7: Effect of particle size on aluminium powder/TNT blending system.

3.3. Effect of gradation of aluminium powder on thermal conductivity of composites

According to the mass ratio of 1:4 for the filling amount of 5wt% spherical aluminum powder, 10μm and 24μm, 20μm and 24μm, 30μm and 24μm particle size grading, according to the mass ratio of 1:1 for the filling amount of 5wt% spherical aluminum powder for the particle size grading of 20μm and 30μm, Figure 8 shows the four groups of different particle size of aluminum powder grading before and after the change of the thermal conductivity of the composite materials schematic diagrams, from the a, b two figures It can be seen that the thermal conductivity of the composites filled with 10μm and 24μm, 20μm and 24μm aluminum powder gradation is higher than that of 24μm alone; from Figure c, it can be seen that the thermal conductivity of the composites filled with 30μm and 24μm particle size gradation is lower than that of both of them; from Figure d, it can be seen that the thermal conductivity of the composites filled with 20μm and 30μm particle size gradation is higher than that of both of them alone; from Figure 8, it can be seen that the thermal conductivity of the composite filled with 30μm and 30μm particle size gradation is higher than that of both of them alone. The thermal conductivity of the composites with 20μm and 30μm particle size grades is higher than that of the two alone. From the simulation results, it can be seen that in the aluminum powder graded filling of different particle sizes, a positive synergistic effect can be produced when graded to a larger particle size with a smaller particle size, and the larger the difference between the particle sizes, the stronger the synergistic effect, which makes the aluminum powder more tightly stacked in the TNT matrix to form more thermal conductivity network, to enhance the thermal conductivity the composite material.

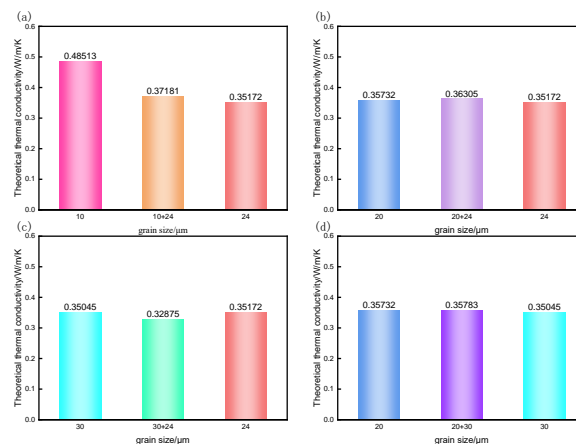


Figure 8: Schematic diagram of thermal conductivity changes of composites before and after grading of aluminium powders with different particle sizes.

4. Conclusions

In this paper, a three-dimensional numerical simulation of thermal conductivity of Al powder/TNT fusion-cast explosives was established to study the site effects of Al powder filling amount, Al powder particle size, Al powder particle size grading, and Al powder morphology on the thermal conductivity of the composite material, and the results show that.

(1) The numerical simulation results agree with the Maxwell-Eucken model results when the particle filling amount is small, and the overall trend is consistent, which can be used to predict the thermal conductivity of Al/TNT composites.

(2) The theoretical thermal conductivity of Al/TNT composites increases exponentially with the increase of the volume fraction of Al.

(3) For relatively low filling amounts (less than 10%) the thermal conductivity of the composites has a tendency to increase and then decrease with increasing particle size of the aluminium powder. For relatively high filling amounts, the thermal conductivity of the composites decreases with increasing particle size of the aluminium powder.

(4) The thermal conductivity of mixed-filled aluminium powder composites is more significant than that of single-filled aluminium powder composites, and the larger the graded particle size, the better the filling effect.

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