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S R. Annapragada

D Sun

S V. Garimella

Purdue University, sureshg@purdue.edu

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Prediction of Effective Thermo-Mechanical Properties of Particulate Composites*

S. Ravi Annapragada, Dawei Sun and Suresh V. Garimella[†]

School of Mechanical Engineering, Purdue University

West Lafayette, Indiana 47907-2088

Abstract

A micromechanics-based model is developed to predict the effective thermo-mechanical properties of energetic materials, which are composite materials made from agglomeration of particles of a range of sizes. A random packing algorithm is implemented to construct a representative volume element for the heterogeneous material based on the experimentally determined particle diameter distribution. The effective mechanical properties of the material are then evaluated through finite element modeling, while its thermal properties are determined through a finite volume approach. The model is first carefully validated against results from the literature and is then used to estimate the thermo-mechanical properties of particular energetic materials. Good agreement is found between experimental results and predictions. The stress-bridging phenomenon in the particulate materials is captured by the model. Thermodynamic averaging is shown to be a poor representation for the estimation of thermo-mechanical properties of these heterogeneous materials.

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Keywords: Effective material properties, Homogenization, Representative volume element, Particulate composites, Granular materials, Explosives

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[†] Corresponding author, Email: sureshg@purdue.edu, Tel: 765-494-5621, Fax: 765-494-0539

1. Introduction

Energetic materials are of significant interest in technological and defense applications in the extraction (mining), structure demolition, space propulsion, and ordnance industries. Increased interest in particulate energetic materials stems from the ability to optimize their performance, burning behavior, stability, detonation properties, and processing characteristics; above all, the low sensitivity of these systems is very attractive [1,2]. A fundamental understanding of the behavior of particulate energetic materials during melt casting is critical in developing improved casting procedures and in the design of novel explosives [3,4,5]. With the enhancement in available computational resources, numerical techniques offer a powerful tool for modeling the thermal/mechanical characteristics of particulate explosives.

The micromechanical behavior of particulate energetic materials has been extensively studied. The stress localization in plastic-bonded explosives (PBX) under different loading conditions was studied by Bardenhagen and Brackbill [6] using the particle-in-cell method. The model was later extended to investigate the internal deformation and grain interaction of granular explosives [7]. A constitutive theory was developed for modeling the mechanical response of dynamically loaded filled-polymer composites based on Mori-Tanaka's effective medium theory [8]. The theory, however, was not applicable to composites with particle concentrations above 30%. An improved model was proposed by Clements and Mas [9] to investigate the mechanical behavior of PBX with a bimodal particle distribution. Using a two-dimensional representative volume element (RVE), Banerjee and co-workers investigated the effective elastic properties of the particulate explosive PBX 9501 [10,11]. In most of these efforts, the random distribution of particles in the unit cell, which is crucial to property prediction, is either ignored [8,9] or manually

controlled [10,11]. In addition, limited attention has been focused on the study of micromechanical properties of explosives other than PBX.

Analytical approaches for estimating effective thermal properties of general particulate composites in the literature were reviewed in Tsotsas and Martin [12]. A recent computational approach by Kumar and Murthy predicts the effective thermal conductivity in a static fluid/solid mixture [13]. This approach alleviates the need for simplifying assumptions on interstitial geometries, a drawback of the analytical approaches [14,15]. The thermal characteristics of explosives, however, have received less attention, and thermal property characterization approaches for these materials have generally been limited to experimental measurements. The large particle loading renders the analysis of the heat transfer behavior of composite explosives challenging.

In the present work, microstructural RVE models are developed to predict the effective thermo-mechanical properties of two composite explosive materials, Composition B and a new formulation, Picatinny Arsenal Explosive (PAX). Random particle distributions were used in generating the appropriate RVEs and the effective property predictions are shown to be RVE-size independent. The predicted effective properties, i.e., Young's modulus, Poisson's ratio, thermal conductivity and specific heat, are compared against available experimental measurements. The heat transfer and stress-localization characteristics of the explosives are also examined.

2. Materials under consideration

The materials studied in this paper, Composition B and Picatinny Arsenal Explosive (PAX), are composites with cyclo-trimethylene-trinitramine (RDX) particles as the particulate filler. Composition B consists of 60%wt RDX and 40%wt TNT [1]. The

PAX material contains >80% wt RDX particles in a matrix of a wax mixture (mainly Carnauba wax). For both materials, the RDX particles are always in a solid state while the TNT/wax matrix experiences solid/liquid phase change during casting. The thermophysical and mechanical properties of RDX, TNT, and Carnauba wax obtained from the literature [16, 17, 18] are listed in Table 1. The thermal conductivity and specific heat of the wax are estimated using thermodynamic averaging. The wax is approximated as an elastic material and a Poisson's ratio of 0.49 is assumed.

3. Microstructure modeling

The RDX particles used in both Composition B and PAX have the same size distribution shown in Figure 1. In order to accommodate the wide range of particle sizes and generate a valid RVE, a multimodal random particle packing algorithm is highly desirable. An efficient methodology for multimodal spherical particle packing was proposed by Lubachevsky and Stillinger [19], and was adopted by Knott et al. [20] to study the combustion behavior of heterogeneous propellants in a cubic RVE. This method is employed in the present work to generate the desired random particle distributions in the RVE with periodic boundaries. The theoretical basis and implementation is discussed in detail in [19] and is not repeated here.

Even though inclusion of a broad range of particle sizes in a RVE would be more representative, the large range of particle sizes causes significant difficulties in grid generation. Thus the actual particle distributions are reduced to three sample particle sizes, as shown in Figure 1. One possible particle distribution in an RVE for Composition B in three and two dimensions is shown in Figure 2 and Figure 3, respectively. Due to the large variation in particle sizes and random distribution of

particles, three-dimensional RVEs containing more than 50 filler particles in general require more than 10 million elements for property prediction calculations. In this study, RVEs with particle counts of 20 and 50 are first considered for three-dimensional computations due to limitations in computational resources. Efforts are then focused on two-dimensional representations in which the effective properties of the particulate media are evaluated using two approaches. In the first (*Method I*), the particle volume percentage in the two-dimensional RVEs is maintained identical to the three-dimensional ones while the particle distribution varies. The efficacy of this simplification has been demonstrated by Banerjee *et al.* [10]. In the second approach (*Method II*), two-dimensional RVEs are generated by slicing the three-dimensional ones along different cross-sections (as shown in Figure 2). Arithmetic averaging over results for different slices and configurations is then used to obtain the effective properties. The validity of this approach is shown in [21]. With the same particle counts, it is evident that particle volume fractions are different among slices in *Method II* whereas different RVEs in *Method I* have the same. It is thus expected that the predicted results given by *Method II* have larger disparities than *Method I* using same RVE sizes even though similar effective values can be predicted.

4. Homogenization methodology

With the packing in a RVE generated and geometry discretized, the macroscopic effective properties of the energetic materials can be evaluated. Since the materials are macroscopically homogeneous, they can be considered to consist of periodic RVEs; thus periodic boundary conditions can be applied. The homogenization scheme utilized for

each effective property prediction, along with the boundary conditions imposed is described below.

4.1 Thermal conductivity and specific heat

For a static RVE with no fluid flow, the following governing equation governs effective thermal conductivity and specific heat capacity:

$$\nabla \cdot (k \nabla T) = \rho c_p \frac{\partial T}{\partial t} \quad (1)$$

For calculating the effective thermal conductivity, the steady-state version of Eq. (1) is solved and a temperature jump ΔT is imposed between the left and right walls of the RVE while the top and bottom walls are assumed to be periodic, as depicted in Figure 3a.

After Eq. (1) is solved numerically, the total heat flux q'' through the left and right side walls are calculated, yielding the effective thermal conductivity:

$$k_{eff} = \frac{q'' L}{\Delta T} \quad (2)$$

For the solution to be considered as a converged result, it is required that

$$\Delta q'' = \left| q''_{left} \right| - \left| q''_{right} \right| < 0.0001 \frac{\left| q''_{left} \right| + \left| q''_{right} \right|}{2} \quad (3)$$

The effective specific heat is evaluated through a two-step approach (Figure 3b). The left wall of the RVE is exposed in the first step to a constant heat flux q'' for time Δt while the other walls are insulated. In the second step, adiabatic boundary conditions are applied to all walls and the RVE is allowed to reach an equilibrium temperature T_e . The effective specific heat is then determined from:

$$c_{p,eff} = \frac{q'' A \Delta t}{\rho V (T_e - T_i)} \quad (4)$$

where A is the area of the left surface and V the volume of the RVE. It may be noted that the accuracy of determination of $c_{p,eff}$ is adversely affected if the choice of Δt is too small; $c_{p,eff}$ obtained from Eq. (4) converges to a constant value as Δt increases. A converged value of $c_{p,eff}$ is achieved if

$$\Delta t \geq \frac{\bar{k}L^2}{\bar{\alpha}} \quad (5)$$

where $\bar{k}$ is the weighted arithmetic mean of the conductivities of the particles and matrix, and $\bar{\alpha}$ is the thermodynamic average of the particle and matrix thermal diffusivities.

For effective thermal property calculations, the commercial software package GAMBIT [22] is used for grid generation, and Eq. (1) is solved with periodic boundary conditions using FLUENT [23]. Quadrilateral finite volumes are used in both two-dimensional approaches, which requires approximately 100,000 nodes for 150-particle RVEs. For the three-dimensional calculations, tetrahedral elements were used for discretizing the computational domain. The resulting RVE with 50 particles contains more than 2 million elements. Numerical simulations were carried out on three sets of successively refined meshes for both two- and three-dimensional RVEs to ensure grid-independence.

4.2 *Young's Modulus and Poisson's Ratio*

Periodicity is imposed on the RVE to mimic the mechanical behavior of a homogeneous medium. Boundary node displacements parallel to the boundary faces are coupled through the following relation:

$$u_i - u_j = 0 \quad (6)$$

where u_i and u_j are displacements parallel to the boundary face of the boundary nodes i and j . The implementation of the periodicity of the RVE is illustrated in Figure 4. As also

shown in the figure, the top boundaries are given a displacement to simulate unidirectional tensile strain. This corresponds to a kinematic uniform boundary condition (KUBC) [24]. Two other prescribed boundary conditions, uniform traction and periodic, have been used in the literature. For a well-defined RVE, Sab [25] showed that once RVE-size independence is reached, effective elastic properties do not depend on the type of boundary condition imposed. Hence the kinematic boundary condition was used due to its ease of implementation. A plane strain assumption was used for the two-dimensional analyses. The stresses and strains in all directions are spatially averaged as:

$$\langle \sigma_i \rangle = \frac{1}{V} \int_V \sigma_i dV \quad (7)$$

$$\langle \varepsilon_i \rangle = \frac{1}{V} \int_V \varepsilon_i dV \quad (8)$$

where i denotes the direction of the stress (/strain) tensor. The two-dimensional Young's modulus and Poisson's ratio are computed as:

$$E_{eff}^{2D} = \frac{\langle \sigma_2 \rangle^2 - \langle \sigma_1 \rangle^2}{\langle \sigma_2 \rangle \langle \varepsilon_2 \rangle - \langle \sigma_1 \rangle \langle \varepsilon_1 \rangle} \quad (9)$$

$$\nu_{eff}^{2D} = \frac{\langle \sigma_1 \rangle \langle \varepsilon_2 \rangle - \langle \sigma_2 \rangle \langle \varepsilon_1 \rangle}{\langle \sigma_2 \rangle \langle \varepsilon_2 \rangle - \langle \sigma_1 \rangle \langle \varepsilon_1 \rangle} \quad (10)$$

The two-dimensional isotropic stress-strain relations are compared against the three-dimensional versions of the equations with a plane strain assumption [26] to obtain three-dimensional elastic properties from the two-dimensional results as follows:

$$\nu_{eff}^{3D} = \frac{\nu_{eff}^{2D}}{1 + \nu_{eff}^{2D}} \quad (11)$$

$$E_{eff}^{3D} = E_{eff}^{2D} \left[1 - \left(\nu_{eff}^{3D} \right)^2 \right] \quad (12)$$

For three-dimensional RVEs, the effective material properties can be evaluated using the constitutive equations as the ratio of corresponding average stresses and strains, which are defined as:

$$\langle \sigma_{ij} \rangle = \frac{1}{V} \int_V \sigma_{ij} dV, \text{ and } \langle \varepsilon_{ij} \rangle = \frac{1}{V} \int_V \varepsilon_{ij} dV \quad (13)$$

In Eq. (13), V is the volume of the RVE, and σ_{ij} , ε_{ij} are the stress and strain components, respectively.

The individual materials of the particles and the matrix in the stress formulation are treated as isotropic. The behavior of an isotropic elastic material is defined by the following differential equation:

$$\frac{\partial}{\partial t} \left(\rho \frac{\partial w_i}{\partial t} \right) = \frac{\partial}{\partial} \left[\mu \left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i} \right) \right] + \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial w_k}{\partial x_k} \right) \quad (14)$$

where $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$ and μ are Lamé's coefficients. ANSYS Mechanical [27] was

used to solve the differential equation above. Eight-node quadrilateral and 10-node tetrahedral elements are used for the two- and three-dimensional mechanical analysis, respectively. The stress-related effective properties (Young's modulus and Poisson's ratio) are then evaluated from the elastic homogenizing technique discussed.

5. Results and comparisons

The RVE elasticity model is first validated against results from the literature. The model is then used to predict the thermo-mechanical properties of Composition B and PAX. The predictions for both materials are compared and validated against available experimental results. The heat transfer and stress-localization characteristics of Composition B and PAX are also briefly examined.

In studying the effective properties of Composition B and PAX, three different particle distributions are examined for each RVE size in *Method I* and five slices are taken from three-dimensional RVEs to construct the RVEs used in *Method II*. The effective values for k , c_p , E and ν are obtained by averaging values from all three arrangements and the standard deviations are presented as the error bars in the corresponding plots.

5.1 Model validation

The benchmark problem considered for validating the RVE model is the prediction of effective elastic properties of a glass-estane composite [10]. The particle concentrations chosen for comparison, 21% and 59%, are the two extrema considered by Banerjee *et al.* [10]. The results are also compared at extrema for strain rates, 0.001s^{-1} and 2400s^{-1} .

The microstructure used in the benchmarking problem contains monodispersed circular particles. A sample distribution is shown in Figure 5. Fixed displacement boundaries corresponding to a unidirectional strain of 1% were imposed as explained earlier. Estane was treated as isotropic with the Young's modulus being a function of temperature and strain rate as summarized in Table 2; a Poisson's ratio of 0.49 was used. The glass beads were modeled as an isotropic material with constant elastic properties over the entire spectrum of strain rates and temperatures considered [10]. A Young's modulus of 50,000 MPa and Poisson's ratio of 0.20 were used for the glass beads.

Figure 6 summarizes the comparisons of the present predictions with those of Banerjee *et al.* [10]. Three sets of results are shown here which cover the extrema of the benchmark problem. The deviations of the present predictions from those presented in [10] are listed in Table 3, with deviation defined as:

$$\varepsilon = \frac{1}{N} \sum_{i=1}^N \frac{|E_{P,i} - E_{B,i}|}{|E_{B,i}|} \times 100\% \quad (15)$$

where N is the total number of temperatures considered for a given case, and subscript “P” and “B” denote the present predictions and data from Banerjee et al. [10], respectively. It is evident from Table 3 that the present results are in good agreement with published results.

5.2 Composition B

The particle distributions in Composition B with different RVE sizes are obtained from the random particle packing algorithm as discussed. Sample two-dimensional RVEs with particle counts of 20, 50, 80, 150 and 250 particles are shown in Figure 7. The corresponding sizes of the RVE are 0.39×0.39 , 0.63×0.63 , 0.81×0.81 , 1.13×1.13 , and 1.46×1.46 , respectively, in mm $\times$ mm.

Thermal conductivity and specific heat

Figure 8 shows the predicted effective thermal conductivity and specific heat of Composition B using the different approaches for various RVE sizes. As mentioned in Section 3, only RVEs with 20 and 50 particles are studied in three dimensions. Also shown in the figure are the upper and lower bounds on thermal conductivity, obtained from idealized series and parallel resistance network, respectively. Experimental measurements from Fedoroff and Sheffield [28] are also shown in the figure. Since $k_{\text{RDX}}/k_{\text{TNT}} \approx 1.1$, an RVE-size-independent value for the effective thermal conductivity is reached with only 20 particles in the RVE. On the other hand, the effective specific heat is seen to feature a stronger dependence on RVE size. At the smaller RVE sizes, the predicted specific heat magnitude varies by more than 14% of the RVE-independent value;

the RVE-independent values are reached with approximately 150 particles in the 2D RVEs. Both *Methods I* and *II* give comparable predictions of the thermal properties, with larger standard deviations observed for *Method II*. This confirms the analysis in Section 3. Results obtained using 2D RVEs are in close agreement with those predicted by the 3D RVEs. The RVE-size-independent predictions for both thermal conductivity and specific heat are seen to match well with the experimental measurements. As the conductivities of the particle and the matrix are comparable, the lower and upper bounds are close and hence either of the bounds can be used as the effective thermal conductivity of the particulate composite. This is not always the case. When the properties of the particle and the matrix differ greatly from each other, the bounds will be far apart from each other and using either would lead to large errors.

Young's modulus and Poisson's ratio

The predicted effective Young's modulus and Poisson's ratio for Composition B as a function of RVE size using the different approaches are shown in Figure 9. The Voigt-Reuss bounds [29] along with the experimentally measured Young's modulus and Poisson's ratio are also shown in the figure for comparison. It is evident from the figure that the two bounds represent a large spread, and using either for the property values would result in significant errors. Predictions from 2D RVEs (by *Methods I* and *II*) and 3D RVEs are in close agreement. The RVE-based predictions, unlike the Voigt-Reuss bounds, match the experimental measurements very well. As the RVE size increases, the variation in predicted effective Young's modulus decreases from an initial value of roughly 10% around the size-independent value, becoming negligible for RVEs with 150 particles or more. The dependence of effective Poisson's ratio on RVE size is minimal. Similar

trends are observed for both *Methods I* and *II*. The predicted RVE-independent Young's modulus and Poisson's ratio for Composition B, as well as experimental measurements are summarized in Table 4.

The discussion above and the results in Table 4 show that reasonable estimations of material properties can be obtained using approaches based on two-dimensional RVEs instead of 3D representations. This is particularly useful in property predictions for highly filled particulate composites with large disparities in particle sizes, for which use of 3D RVEs would be computationally demanding.

5.3 *Picatinny Arsenal Explosive (PAX)*

The results for Composition B above showed that RVE size-independent results are obtained for an RVE with 150 particles. An RVE size-independence study was also conducted for the thermal and mechanical property prediction of PAX as shown in Figure 11 and Figure 12, respectively. The standard deviations for thermal conductivity and Young's modulus for the 150-particle-RVE are 0.16% (0.35%) and 1.4% (4.3%) with *Method I* (*Method II*), confirming that a 150-particle RVE is adequate for the study of PAX as well.

The predicted thermo-mechanical properties using this microstructure are listed in Table 5. The thermal conductivity and specific heat were experimentally measured at Picatinny Arsenal. The numerical predictions again show good agreement with the experimentally measured thermal properties.

5.4 *Comparison of Composition B and PAX*

The thermo-mechanical behavior of Composition B is different from that of PAX due to the differences in their composition. A comparative study of the temperature and stress

fields in the two composite materials is informative. The comparison of the stress contours provides only a qualitative comparison. The actual temperature fields and stress localization in the composites would be different due to the three-dimensional nature of the particulate composites. The transient temperature contours in a 150-particle-RVE of both Composition B and PAX at two different times are shown in Figure 13. A nondimensional temperature of $\theta = 0$ is applied to the top surface of the RVE while the bottom surface is kept at $\theta = 1$. Periodic boundary conditions are assumed for the sidewalls. The Fourier number $Fo = \alpha t/L^2$ is defined based on the effective thermal properties. Even though the average heat penetration depths for the two materials at a given Fo are similar, the temperature distributions are different. One-dimensional heat transfer is observed in Composition B (Figure 13a-b) due to the similarity in thermal diffusivities of RDX particles and TNT ($\alpha_{TNT}/\alpha_{RDX} \approx 1.2$). The temperature contours in PAX, on the other hand, show a more two-dimensional behavior (Figure 13c, d) with a larger temperature drop in the RDX particles. This is due to the greater difference in thermal diffusivity (Table 1) between the filler and matrix in PAX ($\alpha_{wax}/\alpha_{RDX} \approx 3.0$). As these property differences increase, as in the case when aluminum powder is added to the particulate explosives, greater temperature non-uniformity would be expected in the RVE. This could render invalid the averaging approaches generally adopted in studying explosives casting [3]. Two-temperature models must instead be used [30].

The stress contours in a 150-particle RVE of Composition B and PAX are shown in Figure 14, in which stress-bridging behavior is observed. The applied force is concentrated through chains of particles. Such stress-bridging is also found in other granular explosives [6]. The force chains in the particulate explosive are seen to be prominent near agglomerations of smaller particles in between larger particles. This

stress-bridging increases the stiffness of the particulate composite by increasing the resistance to deformation at these chain locations. The stress-bridging phenomenon is more prominent in PAX due to the higher particle concentration and lower stiffness of the binder wax as compared to TNT (Figure 14).

6. Conclusions

Micromechanics-based RVE models are developed for the comprehensive prediction of thermo-mechanical properties of particulate energetic materials with high particle concentrations. The model is applied to predict the thermal conductivity, specific heat, Young's modulus and Poisson's ratio of Composition B and PAX. A multimodal random particle generation algorithm is implemented to generate the microstructure of the particulate composites. An RVE size of $0.81 \text{ mm} \times 0.81 \text{ mm}$ is shown to give accurate, RVE size-independent results for the RDX particle-based materials under consideration. The predicted properties agree very well with experimental measurements. Voigt-Reuss bounds are shown to be inadequate for effective property prediction. For two-dimensional predictions, approaches using RVEs generated based on identical effective particle volume fractions (*Method I*) and slicing three-dimensional RVEs (*Method II*) yield comparable results for both effective thermal and mechanical properties. Properties of particulate composites can be estimated using 2D RVEs instead of 3D RVEs to avoid the complex mesh generation and significantly greater computational time for the latter. Microscopic effects such as stress-bridging in particulate explosives and inhomogeneous thermal behavior specific to PAX are captured using the RVE model developed. In general, PAX with its higher particle concentration is seen to show stronger stress-bridging compared to Composition B.

The microstructural model developed can be extended to predict other properties of the material such as the linear coefficient of thermal expansion (CTE) and electrical conductivity of particulate composites. Prediction of CTE, however, requires new correlations to extend the two-dimensional RVE predictions to particulate composites which are three-dimensional in nature. The current model assumes the material to be isotropic. Material models such as those accounting for visco-elasticity can be included to predict the dynamic response of materials such as wax. These enhancements and extensions to the model are currently underway.

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Figure 1. Experimental particle size distribution of RDX and the sampling used.

Figure 2. Sample particle distributions in (a) three-dimensional RVEs of Composition B. The two-dimensional RVEs taken from (a) at different locations are shown in (b). (L is the length of the RVE.)

Figure 3. Illustration of methods used in the determination of (a) effective thermal conductivity, and (b) specific heat. The two panels in (b) show the two steps involved in the calculation.

Figure 4. Illustration of method used in the determination of effective Young's modulus and Poisson's ratio.

Figure 5. Sample particle distribution of monodispersed circular particles used for benchmarking.

Figure 6. Comparison of predicted Young's modulus with results of Banerjee *et al.* [10] for different particle concentration and strain rates (a) 0.001 s^{-1} , and (b-c) 2400 s^{-1} .

Figure 7. Sample two-dimensional particle distributions in the RVE of Composition B with varying numbers of particles.

Figure 8. Comparison of predicted (a) effective thermal conductivity and (b) specific heat of Composition B for different RVE sizes against experimental values.

Figure 9. Comparison of predicted (a) effective Young's modulus and (b) Poisson's ratio of Composition B with varying RVE size against experimental values.

Figure 10. The three 150-particle RVE configurations (Method I) used for evaluating properties of PAX.

Figure 11. RVE size-independence study of thermal conductivity for PAX.

Figure 12. RVE size-independence study of (a) Young's modulus, and (b) Poisson's ratio for PAX.

Figure 13. Temperature contours at $Fo = 3.74 \times 10^{-2}$ (a, c) and $Fo = 7.48 \times 10^{-2}$ (b, d) in a 150-particle-RVE of (a-b) Composition B and (c-d) PAX.

Figure 14. Von Mises stress distribution in a 150-particle RVE of (a) Composition B, and (b) PAX.

Table 1. Properties of materials used in the present study.

<i>Property</i>	<i>RDX</i> [16]	<i>TNT</i> [17]	<i>Wax</i> [18]
Young's modulus, E (GPa)	18	5.4	1.81 (23°C), 0.77 (37°C)
Poisson's ratio, ν	0.22	0.33	0.49
Density, ρ (kg/m ³)	1800	1560	951
Thermal conductivity, k (W/m-K)	0.29	0.26	1.03
Specific heat, c_p (J/kg-K)	1260	1062	2832
Thermal diffusivity, α (m ² /s)	1.29×10^{-7}	1.57×10^{-7}	3.82×10^{-7}

Table 2. Young's modulus of estane [10].

	<i>Temp (°C)</i>	<i>Modulus (MPa)</i>
0.001s ⁻¹	-40	727
	-30	267
	-20	9.3
	-5	7.5
	23	5
2400s ⁻¹	-40	6250
	-30	4000
	-20	2816
	0	2469
	22	2439

Table 3. Deviation of Young's modulus predicted by the present model from Banerjee et al. [10] for different cases.

<i>Glass percentage (%)</i>	<i>strain rate (s^{-1})</i>	ε
21	0.001	12.0%
21	2400	9.3%
59	2400	2.4%

Table 4. Comparison of predicted effective properties of Composition B against experiments.

<i>Property</i>	<i>Experimental</i> [28]	<i>Numerical</i>		
		2D RVE		3D RVE
		Method I	Method II	
Young's modulus, E (GPa)	10.90	10.46	10.10	10.60
Poisson's ratio, ν	0.29±0.04	0.28	0.28	0.27
Thermal conductivity, k (W/m-K)	0.28	0.28	0.28	0.28
Specific heat, c_p (J/kg-K)	1215	1208	1206	1210

Table 5. Comparison of predicted effective properties of PAX against experiments.

<i>Property</i>	<i>Experimental</i>	<i>Numerical</i>		
		2D RVE		3D RVE
		Method I	Method II	
Young's modulus, E (GPa)	N/A	9.62 (23°C), 6.42 (37°C)	9.46 (23°C), 6.35 (37°C)	9.85 (23°C), 6.60 (37°C)
Poisson's ratio, ν	N/A	0.38 (23°C), 0.40 (37°C)	0.40 (23°C), 0.43 (37°C)	0.39 (23°C), 0.41 (37°C)
Thermal conductivity, k (W/m-K)	0.43	0.44	0.42	0.44
Specific heat, c_p (J/kg-K)	1354	1296	1308	1311