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A Numerical Study of Thermal Conductivity in Polypropylene Composites: Exploring the Synergy of Solid Glass Beads and Ceramic Beads as Fillers

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Abstract

Robust thermal insulation plays a vital role in promoting energy efficiency across various industries. Polypropylene (PP) is economical and easy to process, its limited thermal conductivity restricts its potential in insulation applications. This study examines the enhancement of PP's insulation capabilities through the incorporation of glass and ceramic beads as fillers. Using Finite Element Analysis (FEA), heat transfer was investigated within a PP matrix composite containing solid glass beads (SGB) and ceramic beads, with the microstructure represented by a 3D sphere-in-cube model across varying filler volume fractions. Analysis focused on the impact of bead quantities on the composite's effective thermal conductivity (k_{eff}), aiming to identify optimal bead ratios for improved insulation. The results showed a significant decrease in thermal conductivity with higher filler content, demonstrating the potential of glass and ceramic beads to improve PP for wide range of insulation applications.

Keywords: Polypropylene, Solid Glass Bead, Ceramic Bead, Effective thermal conductivity.

1. Introduction

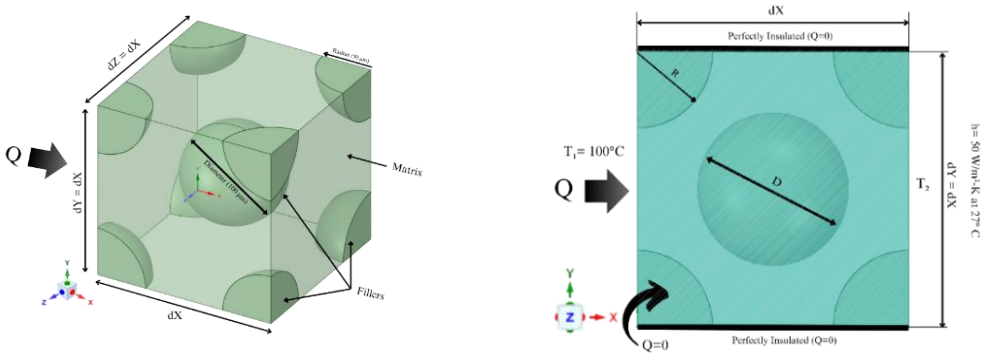
Polypropylene (PP) is popular for applications due to its cost-effectiveness and ease of manufacturing, offering good mechanical properties. However, pure PP has limited thermal insulation capability because its thermal conductivity is higher than desired for effective insulation. As a result of this issue, glass and ceramic beads are introduced in this study to improve PP composite's thermal insulation capability by lowering overall thermal conductivity. Researchers have investigated different methods to enhance the thermal performance of polypropylene (PP) by incorporating solid glass beads (SGBs) as reinforcement, focusing on their composition and their influence on insulation. These lightweight composites offer improved insulation properties, making them ideal for applications such as food storage containers, thermos flasks, insulating panels, and electronic packaging [1]. Mishra et al. [2] employed finite element modelling (FEM) to demonstrate a parabolic decrease in effective thermal conductivity with an increasing SGB volume fraction. Their finding highlighted the potential of SGBs for thermal insulation. Several studies have explored methods to optimize the thermal performance of glass bead reinforced PP composites. Some research [3–5] examined the influence of filler volume fraction on thermal conductivity showing a decline as the filler content increases. Niazi et al. [6] investigated the thermal behavior of polyester resin filled with glass bead fillers, suggesting that for different particle diameters, the coefficient of thermal conductivity depends primarily on weight fraction and not particle size. Surface treatment of SGB emerged as a crucial factor influencing adhesion and compatibility with the PP matrix. Mutua et al. [7] demonstrated superior adhesion and enhanced heat insulation using *NaOH*-treated Glass Beads, also known as hydroxylated glass beads. Tskemess et al. [8] proposed using spherical beads with diameters around one hundred microns as optimal for thermal insulation, emphasizing the dependence of particle size and surface treatment on this application. In a study by Liu et al. [9], it was found that graphene-wrapped fillers can change from insulators to conductors due to the inherent electrical properties of graphene. This study highlighted the sensitivity of thermal conductivity to filler type and composite structure. Research efforts evaluated the significance of precise thermal conductivity prediction models for ceramic-filled polymer composites by investigating the impact of interfacial heat transfer resistance. Feng et al. [10] explored the ability of spherical fillers in polypropylene composites to deflect heat flow. The team's work also emphasized the need to balance thermal insulation with mechanical properties by optimizing the spherical filler content. Incorporating inorganic microspheres into polymer composites complicates heat transfer, so optimizing filler content, surface treatment, and size distribution is crucial for balancing thermal performance.

This study assesses polypropylene composites with varying glass and ceramic bead amounts, focusing on thermal conductivity, microstructure, and filler optimization. Findings will clarify how composite composition and microstructure affect thermal insulation, guiding the development of advanced, high-performance materials.

2. System Modelling

2.1 Physical Modelling

Accurate prediction of composite properties necessitates a comprehensive understanding of microstructure. This study employs a simplified, periodic, body-centered cubic model to investigate the thermal behavior of composites with varying filler volume fractions up to 22.5%. The composite material presumed to be homogeneous, isotropic, and free from voids, with ideal interfacial heat transfer between the components.



(a) (b)

Fig. 1. (a) A sphere within a cube model, occupying 17.9% of the overall volume (b) Two-dimensional view of the model with proper boundary conditions.

The cubic model's conductive path length, *dX*, is uniform across dimensions. A 100-micrometer particle diameter is used, reflecting average commercial fillers. The FEM software, ANSYS 2020 R1, is used to investigate the current study and adjusted *dX* automatically based on filler content. Accurate composite property estimation is crucial for effective design, with microstructure being key. This study assumes a homogeneous composite with isotropic filler, no thermal contact resistance, and a void-free lamina. The filler is systematically arranged in a square periodic layout. A three-dimensional (3D) body-centered cubic Representative Volume Element (RVE) model is used to assess the thermal conductivities of polypropylene composites with glass and ceramic beads at up to 22.5% volume fraction.

2.2 Mathematical Modeling

To study the case, several assumptions were made: a 3D RVE with dimensions of *dX*, isotropic properties of the matrix and the filler, steady state heat conduction, no heat generation inside the RVE and periodic boundary conditions. In the 3D temperature field, the temporal variation of temperature, $T(x, y, z, t)$, within an infinitesimal volume is governed by the heat equilibrium equation. This equation establishes a balance between the heat energy absorbed by the volume and the heat generated within it:

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}+\frac{q}{k}=\frac{1}{\alpha}\frac{\delta T}{\delta t}, \tag{1}$$

where T represents the temperature (K); q is the heat flux (W/m^2); k is thermal conductivity (W/m-K); α is the thermal diffusivity (W/m^2-K); t is the time for conduction of heat (s). These distinct sets of boundaries and initial conditions are employed for the heat conduction analysis, where heat conduction along z-direction is zero. Boundary Condition 1: $T\big|_{x=0}=T_1$ and $T\big|_{x=0}=\phi(x,y)$, where T_1 denotes the initial temperature in Kelvin, and $\phi(x,y)$ represents the temperature distribution function. Here T_1 = 373 K. Boundary condition 2: Convection co-efficient, h = 50 W/m^2-K at 300.16 K is applied to the exposed face. The Fourier law of conduction is employed to evaluate the thermal conductivity, the derived form of Fourier law is as follows:

$$k_{eff} = -\frac{Q}{A}\frac{dx}{dT}, \tag{2}$$

where k_{eff} denotes the composite's effective heat conductivity (W/m-K), Q (W) is the heat flowing through the RVE that is evaluated by FEM software, dx (m) is the length of the conduction, dT denotes the difference in temperature between T_1 and T_2 (K) and A is the cross-section area at which heat flow occurs (m^2).

The viability of applying composites with different formulations of fillers is also evaluated based on these parameters 1) Performance Index (PI) and 2) Price to Performance Ratio (P-P Ratio). The objective of this research is to analyze thermal properties such as effective thermal conductivity and heat flux. The expression for Performance Index and Price to Performance Ratio are as follows:

$$Performance\ Index = W_1.TC_{Norm} + W_2.HF_{Norm}, \tag{3}$$

$$Price\ to\ Performance\ Ratio = \frac{\text{Price}_{Norm}}{\text{PI}}, \tag{4}$$

In (4) weighting factors, W_1 and W_2, are assigned to thermal properties. Thermal conductivity (W/m-K) is attributed a weight of $W_1 = 0.7$, while heat flux (W/m^2) is assigned a weight of $W_2 = 0.3$. The sum of these weights equals one, with the more critical property receiving a higher weight. Normalized values for thermal conductivity (TC_{norm}), heat flux (HF_{norm}), and overall production cost ($Price_{Norm}$) are calculated for the dataset. The general expression for these parameters is as follows.

$$X_{Norm} = \frac{X - X_{\min}}{X_{\max} - X_{\min}}. \tag{5}$$

The equation (5) is used to normalize the thermal conductivity, heat flux, and overall production cost, where X_{norm} represents the normalized value, X is the variable of interest, and X_{min} and X_{max} are the minimum and maximum values of X in the data set, respectively.

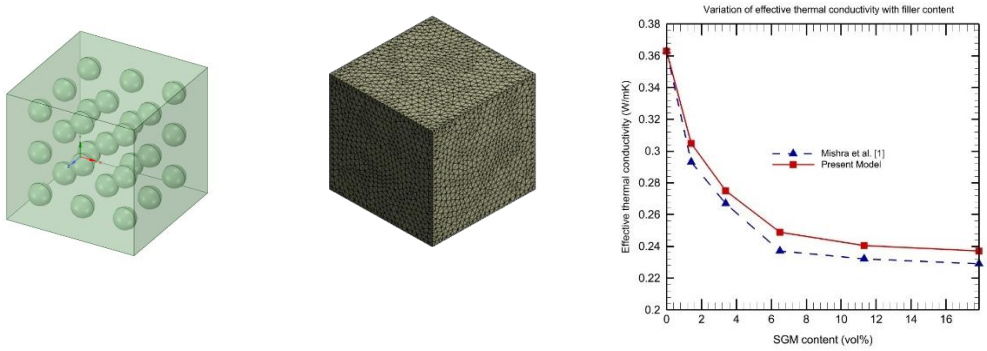
3. Numerical Simulation and Validation

In the current work, a finite element method-based software is utilized to solve the mentioned governing equations utilizing adequate boundary conditions. Heat propagation through the composite material is simulated using the 3D RVE. For both validation and the ongoing investigation, the 3D RVE model is meshed using a triangular unstructured mesh element. An element size of one micron is applied for each volume fraction percentage. As the RVE sizes varied, the mesh element counts also exhibited variation, as detailed in Table 1. & Table 2.

For model validation, the work of Mishra et al. [1] is regenerated. Steady-state heat conduction is modeled with 373 K on one face and convective heat transfer on the opposite, with adiabatic conditions on other surfaces. The model assumed a homogeneous, isotropic material with perfect interfacial contact and square filler arrangement. Epoxy and Glass had thermal conductivities of 0.363 W/m-K [1] and 0.17934 W/m-K [11], respectively. The geometric model included spherical objects dispersed in a cubic matrix.

Table 1. Set up data and comparison of FEA and experimental thermal conductivity [1]

Sample	Matrix	SGB (%vol)	Mesh element type	No. of mesh elements	Avg. flux (W/m^2)	Temp. diff. (K)	k_{eff} (FEM)	k_{eff} (Exp)	% Error
1	Epoxy	0	Triangu-lar Unstructured	1953125	1685.7	5.573	0.363	0.363	0.00
2		1.4		206244	1652.7	3.244	0.305	0.293	4.10
3		3.4		154319	1229.5	6.913	0.275	0.267	3.00
4		6.5		132600	1238.7	5.756	0.267	0.237	5.06
5		11.3		116120	1238.9	4.965	0.237	0.232	3.66
6		17.9		103762	1242.8	4.423	0.229	229	3.49



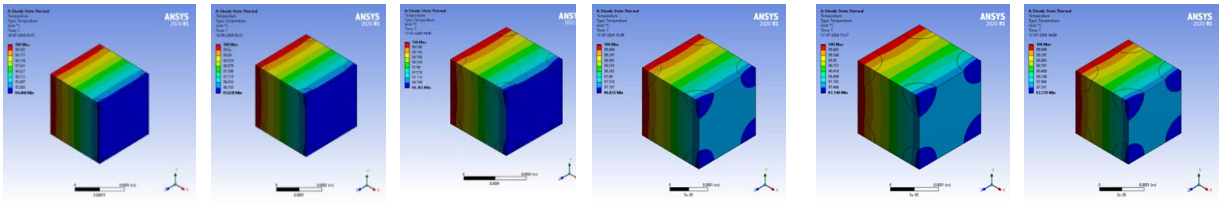
(a) (b) (c)

Fig. 2. (a) A 3D cubic model incorporating spherical inclusions with a volume fraction of 6.5%. (b) A meshed 3D cubic model with triangular mesh elements (c) Variation of effective thermal conductivity with filler content.

The results presented in Fig. 2(c). shows that the current model results are in good agreement with the experimental model, indicating the validation of the experimental model and hence the current research study. However, there is a slight displacement between the two graphs. The discrepancy between simulated and measured conductivity values stems from assumptions in numerical analysis that do not fully represent real conditions. For instance, the simulation assumes an orderly distribution of solid glass beads (SGBs), while the actual composite has a random dispersion in the resin. Additionally, the hardener was omitted from the simulation due to technical complexities. However, the low percentage error gives confidence in the methodology used in our current investigation to closely estimate the thermal conductivity values.

4. Results and discussion

By constructing a Body Centered Cube (BCC), the microstructure of composite materials is simulated using three-dimensional physical models at six separate filler concentrations to facilitate thermal analysis. Further, finite element program, ANSYS is used to numerically estimate the thermal conduction capabilities of these polypropylene composites packed with glass and ceramic up to 22.5% by volume. A systematic investigation is conducted with filler compositions ranging from pure glass to pure ceramic in 25% increments. The results are summarized in Table 2. The thermal conductivities for Polypropylene, Glass, and Ceramic were 0.363 W/m-K [1], 0.17934 W/m-K [1], and 0.12 W/m-K [12], respectively. Fig. 3. illustrates temperature distributions for filler contents of 1.4%, 3.4%, 6.5%, 11.3%, 17.9%, and 22.5%, it also shows that as filler content increases, the temperature gradient indicates an improved ability of the composite to resist heat flow, highlighting the enhanced thermal insulation provided by the fillers. This effect is slightly at the microscale level RVE; however, it becomes more pronounced at the macroscale, where the suppression of heat flow is significantly amplified.



(a) (b) (c) (d) (e) (f)

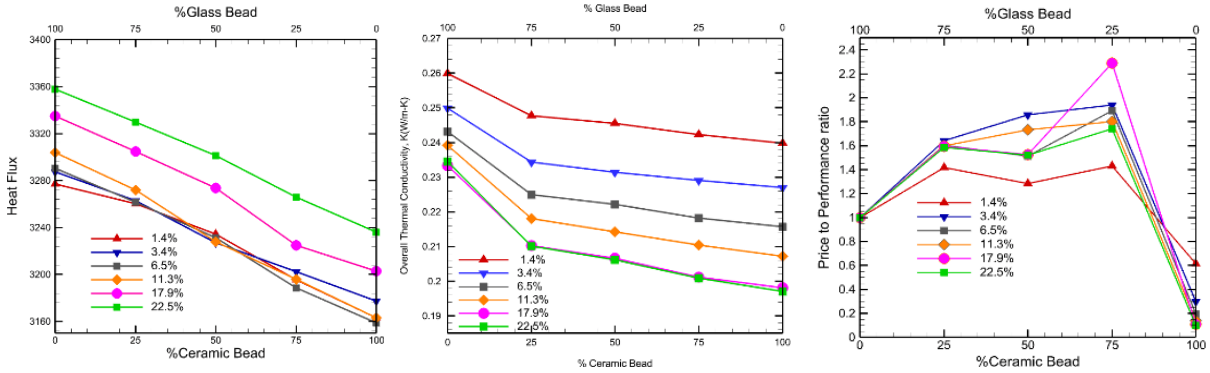
Fig: 3. Temperature profiles for composite with particle concentration of: (a) 1.4 vol.%, (b) 3.4 vol.%, (c) 6.5 vol.%, (d) 11.3 vol.%, (e) 17.9 vol% (f) 22.5 vol% (with a composition of 50% ceramic beads and 50% glass beads evenly distributed in polypropylene material).

Table 2. Thermal conductivity, heat flux, and price-to-performance ratio across various ceramic and glass bead combinations for each volume fraction.

Volume fraction (%)	SGB vol%	Ceramic vol%	Number of mesh elements	Average heat flux (W/m^2)	dT (K)	dX (mm)	k_{eff} (W/m-K)	Cost/kg ($)	P-P Ratio

	100	0		3277	6.0		0.260	5.33	1.000
	75	25		3260	5.3		0.248	5.32	1.416
1.4	50	50	2642019	3235	5.5	0.42	0.246	5.31	1.285
	25	75		3196	5.5		0.242	5.30	1.431
	0	100		3163	5.5		0.240	5.28	0.588
	100	0		3288	4.1		0.250	5.48	1.000
	75	25		3263	4.3		0.234	5.45	1.641
3.4	50	50	1792935	3227	4.3	0.31	0.232	5.43	1.858
	25	75		3202	4.3		0.229	5.40	1.940
	0	100		3178	4.3		0.227	5.37	0.288
	100	0		3291	3.4		0.243	5.70	1.000
	75	25		3261	3.6		0.225	5.65	1.605
6.5	50	50	1413817	3232	3.6	0.25	0.222	5.60	1.511
	25	75		3188	3.7		0.218	5.55	1.893
	0	100		3159	3.7		0.216	5.49	0.188
	100	0		3304	2.9		0.293	6.02	1.000
	75	25		3272	3.2		0.218	5.93	1.600
11.3	50	50	1196868	3228	3.2	0.21	0.214	5.84	1.731
	25	75		3196	3.2		0.210	5.76	1.800
	0	100		3163	3.2		0.207	5.67	0.134
	100	0		3335	2.6		0.233	6.37	1.000
	75	25		3305	2.8		0.210	6.20	1.596
17.9	50	50	1077387	3274	2.9	0.18	0.207	6.09	1.525
	25	75		3225	2.9		0.201	5.97	2.289
	0	100		3203	2.9		0.198	5.85	0.107
	100	0		3358	2.4		0.234	6.48	1.000
	75	25		3330	2.7		0.210	6.35	1.586
22.5	50	50	1018816	3301	2.7	0.17	0.206	6.21	1.522
	25	75		3266	2.8		0.204	6.08	1.739
	0	100		3236	2.8		0.197	5.94	0.099

Surfaces facing the heat flow are presumed to be adiabatic. Nodal temperatures within the domain are computed numerically with Fig. 3. highlighting the behavior of a 50% ceramic and 50% glass mixture in polypropylene matrix.



(a) (b) (c)

Fig. 4. Variation of (a) heat flux (W/m^2) (b) effective thermal conductivity, k_{eff} (W/m-K) (c) Price to Performance Ratio with respect to different mixtures of glass and ceramic bead for different volume fractions.

Fig. 4 (a). shows the heat flux distribution as a function of filler content and the filler volume fraction. The graph clearly demonstrates that the heat flux characteristics at filler concentrations of 17.9% and 22.5% deviate significantly from those observed at other filler content percentages, indicating distinct thermal behavior at these specific levels. Fig. 4 (b). shows these samples' thermal conductivities, which are quite consistent with the

increment of the sample's ceramic beads. Increasing filler content results in more densely packed structures, which enhances the ability to suppress heat flow and thereby reduces thermal conductivity. A percolation effect is observed once the filler content exceeds 17.9%. The presence of a percolation effect is detected when a certain quantity of filler is added, beyond which the heat conductivity of the composite remains unchanged. To make the comparison of the cost's effectiveness possible, Fig. 4(c). shows an assessment that can be quantified of the value that specific composite configurations offer in terms of price for the performance achieved. The cost of making the composite as shown below is estimated using genuine prices sourced online. Polypropylene costs $1.2/kg [13], Glass $4.25/kg [14], and Ceramic $3.00/kg [15]. Fig. 4 (c). also depicts the relationship between the percentage of mixed filler content and the cost effectiveness of the developed composite material. The non-linear appearance discloses that at some concentrations of this filler, the data shows an inconsistent trend, with thermal conductivity exhibiting both increases and decreases at various filler concentrations. The maximum efficiency is achieved with a 100% ceramic bead combination, providing the lowest thermal conductivity for each volume percentage of filler, offering the best price-to-performance ratio, and making it a cost-effective choice for optimal thermal insulation. A lower price-to-performance ratio indicates that the composite delivers better performance relative to its cost. However, the use of 100% ceramic or 100% glass beads in polypropylene composites is constrained by manufacturing feasibility problems such as inadequate dispersion and tool wear. Ceramic beads increase brittleness, while glass beads, though more expensive compared the ceramic beads, compromise mechanical strength. A 50% glass bead - 50% ceramic bead mix in polypropylene achieves a better balance between cost, performance, and production feasibility, making this configuration a more realistic option for real-world applications. Future research may optimize these filler combinations to improve thermal and mechanical qualities while addressing production restrictions.

5. Conclusion

The investigation into the thermal conductivity of glass and ceramic bead-filled PP composites found that: Glass and ceramic beads effectively reduce PP's thermal conductivity, with a 1.4% filler volume decreasing it by 14.3% and 17.9% filler reducing it by 33.15%. Thermal conductivity improves with filler until a continuous network forms at 17.9% filler; beyond this, additional filler has negligible effect. At elevated filler concentrations, a percolation effect becomes evident. Beyond this point, additional fillers fail to enhance thermal insulation and may, in fact, compromise the mechanical integrity of the composite. These lightweight composites offer enhanced insulation properties, making them well-suited for various thermal insulation applications.

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