Research Article

Mechanics of Materials Natural Fibers Technology on Thermal Properties of Polymer

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The thermal characteristics of polymathic methacrylate combined with unsaturated polyester were determined by numerical and experimental research. Models for numerically investigating the parameters of thermal conductivity, specific heat capacity, and thermal diffusivity were developed using COMSOL Multiphysics. The numerical data were then compared to experimental results for the same material using the same measurements to ensure that they were correct. By comparing the thermal conductivity data to two sets of theoretical data, the results were confirmed. The COMSOL models were quite close to the experimental data, with just minor differences between the three models. One set of theoretical data coincided with the mean of the other data, while the second set revealed a significant departure below the other data.

1. Introduction

Despite the fact the polymer composites have been around for a long time, novel composites have been produced in the recent few decades and used in a variety of demanding applications [1]. The synthetic apparatus of today's polymer composites relies heavily on polymer mixtures. They are often manufactured by combining two or more polymers to create a miscible mixture with much better physical qualities than the separate polymers. Polymer blends may be used in a wide spectrum of material processing and manufacturing because of their distinct properties [2, 3]. The majority of polymer blends are made by mixing molten polymers to create heterogeneous systems with an emulsion structure. The component with the smaller volume fraction is disseminated in the medium of the second piece

as particles. Thermal characteristics of polymer blends are highly prized because they can give crucial information regarding their functioning in many applications [4]. Furthermore, data on thermal characteristics can aid in identifying the best processing settings and heat transport studies of the nominated materials [5, 6]. Thermal conductivity, thermal diffusivity, and specific heat capacity are important examples of the thermal qualities that need to be understood for these materials, because this knowledge may assist designers and manufacturers make sound judgments about whether or not to employ them in the intended applications. Such investigations and methods need a thorough understanding of the heat flux profile, which is based on the creation and refinement of highly effective models that can precisely anticipate thermal behavior [7].

To anticipate the thermal characteristics of polymer composites, several theoretical and experimental studies have been undertaken [8]. However, just a few researches have attempted to simulate polymer mixes. Because it incorporates complicated geometrical and thermodynamic principles, both in terms of their reactions to thermo-mechanical stresses and with regard to the mechanics of miscibility itself, modeling polymer blends necessitates tremendous attention, thinking, and focus. Furthermore, because of their complexity, generating successful models of polymer blends needs a fast computing environment capable of handling the vast number of items in the finite element mesh. All load and boundary conditions contained in the model domains should be computed and solved using the CAD (Computer Aided Design) system.

The finite element technique is a systematic approach for converting functions in an infinite dimensional function space to finite dimensional function space and then to ordinary vectors (in a vector space) that may be solved numerically.

COMSOL Multiphysics is well-known as a reliable finite element analysis program. Its sound and user-friendly architecture, as well as its capacity to permit highly exact theoretical studies, have made it the preferred analytical program for a variety of physical issues, including thermal and structural characterizations [9]. Polyamides are among the most widely used crystalline engineering thermoplastics, owing to their outstanding performance features such as high melting temperatures, high mechanical strength, and excellent solvent resistance [10]. PMMA (polymethacrylic methacrylate) is a transparent polymeric material with a number of desired features, including low weight, high transparency, chemical resistance, weathering corrosion resistance, and good insulating capabilities. When it comes to composites and polymer blends, unsaturated polyester (UP) is one of the most useful polymers [11–13].

The features of these blends may be easily studied and investigated using the modeling method, and it is critical that each model undergoes a highly reliable and efficient experimental validation. Estimating the characteristics of polymer blends can aid in making more accurate predictions regarding their behavior.

The several types of polymer blends explored in this study were made up of the two polymers mentioned above: UP and PMMA. In terms of polymer volume fractions and geometrical constructs, the two models differed. Their thermal characteristics were studied, including thermal conductivity (k), specific heat capacity (C), and thermal diffusivity.

1.1. Thermographic Analysis. Thermal analysis was carried out in two ways. The first included theoretical techniques based on Maxwell's theory [14, 15], which employs a unique equation to calculate the thermal conductivity of a polymer-and-distributed-filler system. The equation is used to calculate the thermal conductivity of polymer blends rather

than polymer and filler systems, in which the UP was utilized as the matrix and the PMMA was employed as the second phase material. The following is the equation:

$$k = k_{UP} \frac{2k_{UP} + k_{PMMA} - 2(k_{UP} + k_{PMMA})\phi_{PMMA}}{2k_{UP} + k_{PMMA} + 2(k_{UP} + k_{PMMA})\phi_{PMMA}}. \quad (1)$$

The appropriate heat conductivities of polyester resin (UP) and polymethacrylic methacrylate (PMMA) are k_{UP} and k_{PMMA} , respectively. In the PMMA:UP composite, PMMA is the mass fraction of PMMA.

The second way for calculating k is to utilize Bridgeman's theory, [12–15] which looks at effective thermal conductivity using a different method based on the modified equation:

$$1 - \phi = \frac{k - k_{PMMA}}{k_{UP}} \left(\frac{k_{UP}}{k} \right)^{1/2}. \quad (2)$$

The second sort of study includes building and investigating three alternative models using Simulation Tool 5.3 and a range of geometric and theoretical principles. These were determined as the best models to employ for this sort of research based on relevant experimental data.

Each component was represented as a circle with a radius corresponding to its volume fraction in the initial model, which was generated using two-dimensional geometries. The volume fractions were changed using a parametric approach. The 2D model was named after it, and it is seen in Figure 1.

The third model, dubbed the 3D model, was created utilizing three-dimensional geometry. This model was created to imitate experimental measurement samples with various volume ratios and a constant thickness of 3 mm (which is consistent with the experimental test sample shape) (Figure 2).

The squared lattice model based upon that Flory–Huggins model was used to construct the third model. A lattice model has the advantage of being the best form of model for dealing with binary mixes of various structures.

The Flory–Huggins model is being utilized for the first time to investigate the thermodynamics of mixing binary systems such polymer blends and/or polymer-solvent mixtures. The lattice model's key benefit is that each material's molecules may explicitly disperse over the lattice squares, allowing each square to be occupied by only one kind of molecule.

The models were solved with the help of thermal conduction considerations using the heat transfer in solids module.

The following were the imposed boundary criteria within the context of these considerations:

- (1) For the 2D model, two distinct temperatures T_1 and T_2 were applied to each quadrant of the outer circle, with T_1 referring to ambient temperature and T_2 referring to raised temperature. To ensure that the test was as exact as feasible, the other two opposing quarters were isolated

FIGURE 1: Surface temperature distribution.

FIGURE 2: Polymer blend volume fraction.

- (2) T_1 and T_2 were applied to the bottom and surfaces of the 3D model, respectively, while the cylinder's side wall was insulated

T_1 and T_2 were used on the left and right walls, respectively, in the F-H model.

The following formula was used to get the numerical value of the effective thermal conductivity:

$$k = \frac{\phi}{A} \frac{R}{(T_1 - T_2)}. \quad (3)$$

Specific heat capacity, in contrast to conductivity, is a measurement of a material's ability to store thermal energy. The thermal diffusivity is the third property in the heat transfer equation, and it depends on the other two characteristics (thermal conductivity k and specific heat capacity at constant pressure C_p) and may be calculated using the following formula:

$$\alpha = \frac{k}{\rho C_p}, \quad (4)$$

where ρ is the density measured in kg/m^3 .

As a result, a material's thermal diffusivity may be defined as the ratio of thermal energy conduction to thermal energy storage.

1.2. The Procedure for Testing

1.2.1. Models of Different Materials. Material models are all mathematical approximations of real-world physical behavior. Material models, on the other hand, are not usually developed from physical concepts such as mass conservation or equilibrium equations. They are phenomenological in nature and based on measurements. The mathematical frameworks of material models and the possible values of material attributes will, however, be constrained by physical laws.

Even in ordinary life, it is commonly understood that different materials behave in radically different ways. A material can be extremely brittle, such as glass, or extremely elastic, such as rubber. The operating conditions, as well as the material itself, play a role in selecting a material model. A typical instructional experiment is to soak a piece of rubber in liquid nitrogen until it becomes as brittle as glass. Additionally, when glass is heated, it begins to creep and exhibit viscoelastic behavior.

The translucent, viscous unsaturated polypropylene resin (UP) from (SIR) employed as one of the study's polymers has a density of 1200 kg/m^3 at ambient temperature. When a hardener (methyl-ethyl ketone peroxide (MEKP)) made by the same business is added to UP, it solidifies (SIR). This polymer, together with methacrylate (PMMA) from Castavia, was combined for 1-2 minutes in an electrical blender to achieve the ratios specified in the modeling. The hardener was then added to the reaction mixture and let to set for 24 hours. The solid composite was then placed in a furnace at 55 degrees Celsius to finish the solidification processes.

The hot disc technique was used to test thermal conductivity, thermal diffusivity, and specific heat capacity. Discussion of the findings agrees with the actual data (as shown in Table 1 and Figure 2). The experimental data differed only little from the COMSOL models, which differed less from one another.

The surface temperature pattern for the three numerical models is shown in Figure 1. In contrast to the 3D sample, where the hot zone prevailed over the model's other regions, the hot region did not dominate the whole model in the 2D sample. The temperature distribution in the F-H model was more uniform. The 2D model had the biggest height fluctuations in temperature, with a rate of 71 percent, while the F-H model had the lowest, with a rate of just 12 percent.

In contrast to the anticipated data from Maxwell's theory, Table 2 which showed substantial variation from the others, all COMSOL models, as well as Bruggeman's theoretical data, showed complete.

This behavior differs in terms of specific heat and thermal diffusivity, where modeling data demonstrate substantial variation for various blend proportions, as

TABLE 1: Surface temperature.

Surface temperature (X)	Y	Z
-0.03	5	250
-0.06	10	300
0	15	350
0.03	20	400
0.06	25	450

TABLE 2: Substantial variation.

TC (W/M.K)	PMMA.UP	Value
0.1	0	0.2
0.2	3	0.3
0.15	6	0.4
0.16	9	0.5
0.17	12	0.6
0.18	15	0.7
0.19	18	0.8
0.1	21	0.9
0.2	22	0.10
0.3	25	0.11
0.4	28	0.12
0.5	29	0.12

illustrated in Figures 1 and 2. However, when it comes to the thermal diffusivity data, both the model and the experimental data exhibit a similar pattern of change.

A comparison of numerical and experimental data for specific heat data as a function of polymer blend volume fraction combines the statistical validation of calculated and measured data from several modeling setups.

The validation evaluations suggest that the COMSOL models and experimental work are generally in excellent agreement and that the differences between the two types of analysis are within acceptable ranges. For each attribute, however, the data deviation is different.

When just one of the two polymers is maintained in the polymer blend, the biggest deviations occur, and when the polymer blend is at the intermediate concentration, the deviations are minimized. At the 15 percent and 20 percent PMMA:UP volume fractions, the Flory-Huggins configuration displays less variation than the others.

Unlike thermal conductivity, the attribute of specific heat follows a distinct pattern. The equilibrium concentration of 15% causes the biggest variation in specific heat, whereas the PMMA content with the lowest PMMA content offers the best agreement between the models and experimental results. The F-H configuration, notably at the 15% and 20% PMMA volume fractions, exhibits the highest agreement with the experimental results.

The deviations for diffusivity and thermal conductivity and specific heat reveal considerable differences. At 20% PMMA:UP, the maximum deviation of the F-H model, the greatest variance in diffusivity arises. As the PMMA concentration climbs from 5% to 15%, the two other models indicate a progressive increase in their departure from the experimental data, before dropping to a lower value at 20% PMMA:UP. The deviation of the F-H model climbs with the

others until it reaches 15% PMMA, UP, when it reduces to a value similar to the lowest PMMA concentration in the PMMA:UP mix. Because the applied loads and boundary conditions were consistent throughout the investigation and across all polymer blend proportions, the data dispersion could be ascribed to differences in design parameters and measurement setups. Geometrical concerns might possibly explain the nonuniform trends in the validation data.

2. Conclusions

According to the validation results, the COMSOL models and experimental work are generally in great agreement, and the differences between the two forms of analysis are within acceptable limits. The data deviation, on the other hand, varies by attribute.

The highest variations occur when only one of the two polymers is kept in the polymer mix, and the deviations are minimized when the polymer blend is kept at an intermediate concentration. The Flory-Huggins configuration exhibits less fluctuation than the others at the 15% and 20% PMMA:UP volume fractions.

Although there are minor differences between the three proposed models, COMSOL appears to function well with polymer mix modeling. The minimal differences in deviation amongst the three models suggest that the model type has little impact on the prediction process. The F-H model, on the other hand, is the most suggested for this investigation.

Overall, COMSOL can be utilized effectively to solve and forecast the behavior of polymer blends when using trustworthy and validated data.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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