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Numerical investigation of the effect of temperature and volume fraction on the thermal properties of polystyrene silver nanoparticle (PS/AgNPs) composites

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Abstract: In this paper, the effect of temperature and volume fraction on the thermal properties of polystyrene silver nanoparticle (PS/AgNPs) composites is numerically investigated. This polymer nanocomposite consists of different quantities of silver (Ag) nanoparticles incorporated in a polystyrene (PS) matrix. The temperature dependence of the core-shell nanoparticles is investigated in the framework of *Maxwell model* and the *Rule of Mixture model* for random nanocomposite. By modeling the nanoparticles as being spherical, the effect of volume fraction and temperature on the core-shell nanoparticles is studied via both models for spherical core-shell nanoparticles. Simulations are successfully carried out using MATLAB programming to account for the effective thermal response which occurs at the wide interface between materials. The results show that the thermal conductivity of the matrix material can be enhanced by embedding high thermal conductivity nanoparticles, but the effectiveness of such a strategy diminishes as the effective thermal response between the nanoparticles and matrix material increases. Further simulations indicate that the enhancement of thermal conductivity can be affected by the alignment of nanoparticles with respect to the temperature gradient. The values obtained from the analytical *Maxwell model* compared to *Rule of Mixture model* are in close agreement with the experimental valuesfor a spherical nanocomposite. The Sufer 16 software is further used to show the 2-D contour of thermal conductivity variation over particle volume fraction and temperature of polystyrene silver nanoparticles (PS/AgNPs) composite. The polystyrene silver nanoparticles composite are expected to have adequate potential for a wide variety of applications particularly in microelectronic industries.

Keyword : *Polystyrene, Silver nanoparticles, Temperature, Thermal conductivity, Heat conduction, Spherical composite*.

1. Introduction

Polymer nanocomposites (PNCs) are materials which have nanoparticles dispersed in a polymer matrix. In this paper, the polystyrene silver nanoparticle (PS/AgNPs) composites which consist of different quantities of silver (Ag) nanoparticles incorporated in a polystyrene (PS) matrix are considered. Polystyrene Silver nanoparticles (PS/AgNPs) composite are increasingly used in various fields, including medical, food, health care, consumer, and industrial purposes, due to their unique physical (optical, electrical, and thermal), chemical and biological properties. The polystyrene silver nanoparticles composite are expected to have adequate potential for a wide variety of applications particularly in microelectronic industries (Jibrin *et al.,* 2019).

In recent times, many experimental research works have been carried out on these composite materials (Zhong, Shan&Lang, 2005),(Cunningham, Huang& Baird, 2007), (Schuster *et al.*, 2008), (Zeng *et al.,* 2009),(Banjare *et al.*, 2014),(Kiran, 2016), (Jibrin *et al.,*2019), as well as theoretical efforts to understand the physics(Maxwell, 1904), (Kandula, 2011), (Blanco-Lopez*et al.,* 2015).

The effective thermal conductivity of the nanocomposite is crucial for their design (Sarmad *et al.,* 2022).It has been observed that many factors such as particle shape, particle position, volume fraction, and temperature may influence the thermal conductivity of PS/AgNPs composites structure and it is very difficult to predict the influence of these factors by experimental process. Moreover, simulations based on solving thermal transport equations, exploring a large parameter space, can be cumbersome and challenging (Thorne *et al.,* 2006).

In this paper, the temperature dependence of the core-shell nanoparticles is investigated in the framework of both the *Maxwell model* (Blanco-Lopez *et al.,* 2015) and the *Rule of Mixture model* (Nadendla, 2019) for random nanocomposite. The nanoparticles are modeled as being spherical while the effect of volume fraction as well as temperature on the core-shell nanoparticles is studied via both models for spherical core-shell nanoparticles. Simulations are alsocarried out using MATLAB programming to account for the effective thermal response which occurs at the wide interface between materials.

2. Theoretical Models and Simulations

Several theoretical and empirical models have been proposed to predict the effective thermal conductivity of composite materials. Many of them predict the thermal conductivity by knowing the filler concentration. Most of the theoretical models provide lower and upper bound values of thermal conductivity. These are mainly useful for relatively lower concentration of filler material (Devpura *et al.,*2001). In this paper, the Maxwell model and the Rule of Mixture model are adapted for simulations using MATLAB programming.

2.1. Maxwell Model

In order to obtain an analytical expressions for the effective thermal conductivity of heterogenic medium, Maxwell (1904) modeled the application of an external temperature field with gradient of magnitude G, through a dilute dispersion of spherical nanoparticles embedded in a continuous Polymer matrix of constant thermal conductivity λ_m containing multiple spherical inclusions of radius r(not necessarily in a regular array) of constant conductivity λ_f. The sizes of the particle inclusions are small relative to the inter-particle distances, so that the thermal disturbances to the temperature field due to each inclusion can be considered independently.

The Maxwell model has been adapted (Blanco-Lopez *et al.,* 2015) in obtaining an expression for the effective thermal conductivity of polymer nanocomposite (PS/AgNPs) as

$$K_{eff} = \lambda_m + 3\phi_V \frac{\lambda_f - \lambda_m}{2\lambda_m + \lambda_f - \phi_V(\lambda_f - \lambda_m)} \tag{1}$$

where ϕ_V is the Volume fraction of the filler material (Ag).

The Maxwell equation takes into account only the particle volume concentration and the thermal conductivities of the particle and base medium.

2.2. Rule of Mixture Model

Rule of mixture model considered material in the form of spherical inclusions arranged in a simple cubic array, embedded in a continuous polymer matrix. In Rule of mixture model, thermal interaction between nanoparticles had been taken into consideration and expression for the effective thermal conductivity of polymer nanocomposite (PS/AgNPs) as:

$$\frac{K_{eff}}{K_m} = 1 + \frac{3\phi}{\left(\frac{K_1 - 2K_m}{K_1 - K_m}\right) - \phi + 1.569\left(\frac{K_1 - K_m}{3K_1 - 4K_m}\right)\phi^{\frac{10}{3}} + \ldots} \tag{2}$$

where, K_1 is thermal conductivity of nanocomposite, and K_m is the thermal conductivity of polymer matrix

2.3. Simulations

The analysis of the heat conduction consists of a spherical nanocomposite enclosed by two concentric spheres. The nanocomposite is made of Ag nanoparticles randomly dispersed in a PS matrix. To compute the effective thermal conductivity of the nanocomposite, the temperature of the PS sphere and Ag enclosing the nanocomposite was set to 1.0 and 2.0, respectively. Maxwell and Rule of Mixture models depend on many factors, such as, temperature of nanoparticles, volume fraction of the nanoparticles and shape/size of nanoparticles. In order to investigate the effect of volume fraction of silver nanoparticles (AgNPs) as fillers material and the effective thermal conductivity(K_{eff})of Polystyrene (PS) as polymer matrix with their varying volume fraction, equation (1) and equation (2) were simulated using MATLAB programming. Then MATLAB simulation code base on their volume fraction ranging from 2.5 to 12.5 % are performed so that the heat conduction in the nanocomposite reaches a steady-state. For validation, the *Maxwell model* predictions and *Rule of Mixture model* are compared to experimental data.

3. Results and Discussion

The thermal conductivity of PS/AgNPs obtained via the *Maxwell model* agrees well with the experimental data for nanoparticles concentrations ranging from 2.5 to 12.5% of volume fraction than when compared with the results via*Rule of Mixture model*. Table 4.2 gives effective thermal conductivity of the Polystyrene Silver nanoparticles (PS/AgNPs) composite for volume fraction ranging from 2.5% to 25%. For a given (PS/AgNPs) of 10 nanoparticles size, the effective thermal conductivity of the (PS/AgNPs) composite material increases as the volume fraction is increasing. The table shows the comparison of effective thermal conductivity of (PS/AgNPs) composite calculated using both models with the measured experimental values.

3.1. Particle Temperature and Volume fraction on Thermal Properties of (PS/AgNPs) Composite

The results of thermal conductivity simulation at different volume fraction and temperatures using both Maxwell and Rule of mixture model are provided in Table 1for the temperature values of 100℃ to 500ºC. It is noticed that increasing the volume fraction from 2.5 % to 12.5 % causes an increase in the thermal conductivity of the composite structure as the function of the temperature for the Maxwell model. This enhancement in thermal conductivity with increasing volume fraction is as a result of the increasing alignment of the dominant heat conducting covalent bonds in each polymer chain with the direction of heat transfer.

Table 1. The thermal conductivity measured at different volume fractions from 100 °C to 500 °C Temperature

Temperature (°C)	Volume Fraction (%)	Effective Thermal Conductivity of Composite K_{eff}(W/mk)		
		Maxwell Model	Rule of Mixture Model	Experimental Values
100	2.5	0.621	0.373	0.620
100	5.0	0.632	0.352	0.631
100	7.5	0.640	0.346	0.643
100	10	0.660	0.340	0.660
100	12.5	0.638	0.336	0.638
200	2.5	0.634	0.321	0.630
200	5.0	0.655	0.347	0.655
200	7.5	0.653	0.356	0.652
200	10	0.674	0.379	0.672
200	12.5	0.682	0.323	0.682
300	2.5	0.652	0.340	0.654
300	5.0	0.666	0.325	0.660

Temperature (°C)	Volume Fraction (%)	Effective Thermal Conductivity of Composite $K_{eff}(W/mk)$		
		Maxwell Model	Rule of Mixture Model	Experimental Values
300	7.5	0.679	0.356	0.677
300	10	0.698	0.348	0.696
300	12.5	0.718	0.321	0.712
400	2.5	0.726	0.311	0.726
400	5.0	0.672	0.320	0.678
400	7.5	0.610	0.341	0.609
400	10	0.707	0.398	0.709
400	12.5	0.695	0.345	0.693
500	2.5	0.693	0.367	0.693
500	5.0	0.683	0.347	0.684
500	7.5	0.843	0.355	0.842
500	10	0.774	0.333	0.770
500	12.5	0.735	0.326	0.731

In the Maxwell model, nanoparticles are assumed to be randomly dispersed in the host polymer matrix. The study of the effective thermal conductivity of nanocomposite in which nanoparticles are aligned with respect to the temperature gradient is considered in two extreme cases. In the first case, applying the Maxwell model for Ag nanoparticles aligned normal to the temperature gradient with PS sphere; while in the second case, the Rule of Mixture is applied for Ag nanoparticles aligned in the temperature gradient direction with PS.

Figures 1 to 5 display the thermal conductivities for (PS/AgNPs) nanoparticles composite as a function of temperature, the dependence of the thermal conductivity on the particle temperature, as well as, that of the increases as the particle volume fraction increases.

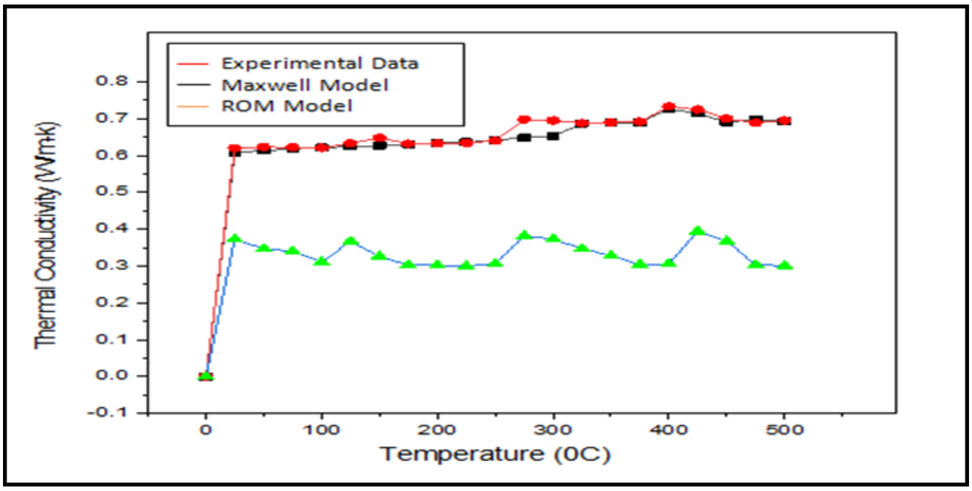

Figure 1. Variation of thermal conductivity of PS/AgNPs with particle temperature obtained for particle volume fraction of 2.5 %

Figure 1 clearly shows a steady increase of thermal conductivity from particle volume fraction of 2.5 %. The value of the thermal conductivity ranges between 0.620 W/m-k to 0.693 W/m-k which correlate that Maxwell model agreed with the experimental data for the temperature variation with volume fraction ranges from 2.5 %. The result show that the thermal conductivity enhancement in PS/AgNPs composite increases as the particle temperature increases. It was observed that while the deviation from Maxwell model prediction is small when nanoparticles are aligned normal to the temperature gradient, the enhancement is substantially stronger when nanoparticles are aligned along the temperature gradient direction (Nguyen *et al.,* 2007).The smaller effective thermal conductivity for vertical alignment case compared to the Maxwell model prediction may be caused by the fact that nanoparticles in such a configuration provide a less efficient heat conduction path way (in the temperature gradient direction) than the Rule of mixture model.

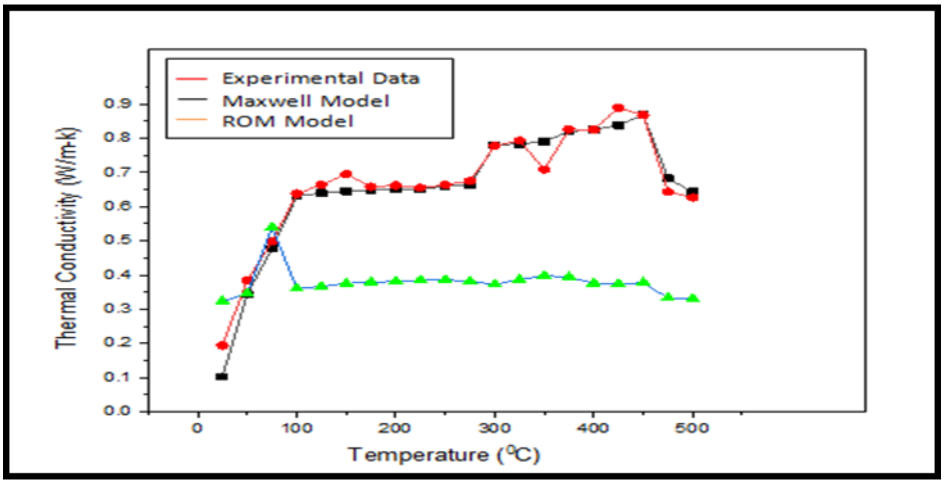

Figure 2. Variation of thermal conductivity of PS/AgNPs with particle temperature obtained for particle volume fraction of 5.0 %

Figure 2 clearly shows a steady increase of thermal conductivity from particle volume fraction of 5.0 %. The value of the thermal conductivity ranges between 0.631 W/m-k to 0.683 W/m-k which correlate that Maxwell model agreed with the experimental data for the temperature variation with volume fraction ranges from 5.0 %. From the graph, it can be seen that as the volume fraction of the nanoparticles increased, the temperature corresponding to maximum thermal conductivity shifts to higher values. For a volume fraction of 5.0%, maximum thermal conductivity is reached at a temperature of 200 °C. Furthermore, as the volume fraction is further increased to 7.5 %, the temperature corresponding to peak thermal conductivity decreases to 100 °C. This temperature corresponding to peak value of thermal conductivity for a volume fraction of 5.0% is lower compared to that for the pure polystyrene polymer by almost 250 °C as shown in Figure 5. This suggest that the volume fraction of AgNPs can be even more effective for thermal management at lower temperatures (Yang& Han, 2006). This is seen by noticing that while at a temperature of 350 °C, drawing the polymer to a volume fraction of 5.0% leads to an increase in thermal conductivity from

0.670 W/m-k to 0.690 W/m-k representing an enhancement of thermal conductivity at the higher temperature of 500 °C.

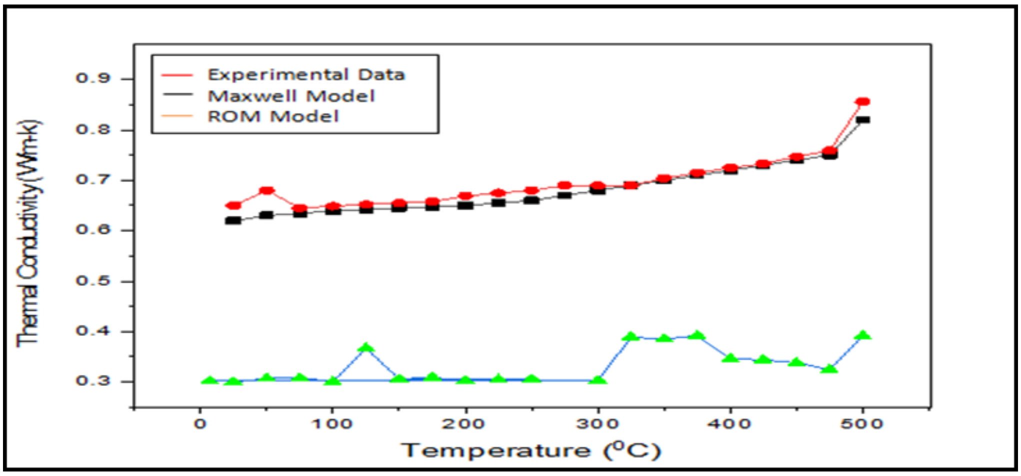

Figure 3. Variation of thermal conductivity of PS/AgNPs with particle temperature obtained for particle volume fraction of 7.5 %

Furthermore, Figure 3 reveals that the temperature distribution inside PS/AgNPs nanocomposite with embedding nanoparticles shows the existence of noticeable temperature inside the simulation domain of PS sphere and that the temperature is relatively uniform inside the Ag nanoparticles, which is consistent with the higher thermal conductivity of the nanoparticles.

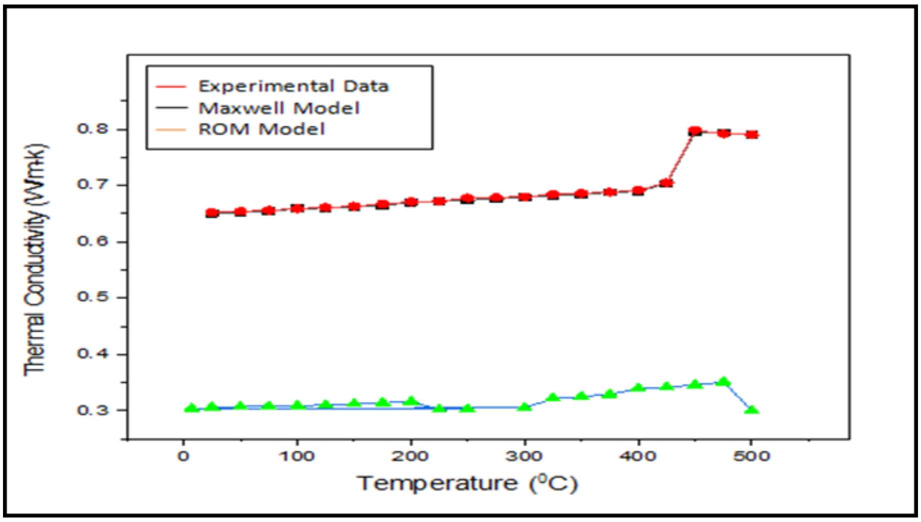

Figure 4. Variation of thermal conductivity of PS/AgNPs with particle temperature obtained for particle volume fraction of 10.0 %

Figure 4 clearly shows a steady increase of thermal conductivity from particle volume fraction of 10.0 %. The value of the thermal conductivity ranges between 0.660 W/m-k to 0.700 W/m-k which correlate that Maxwell model agrees with the experimental data for the temperature variation with volume fraction ranges from 10.0 %. The result show that the thermal conductivity enhancement in PS/AgNPs composite increases as the particle temperature increases. The Maxwell's model can predict the dependence of the thermal conductivity on temperature for all nanoparticles volume fraction and types and this is shown that the smaller effective thermal conductivity of the nanoparticles the higher the temperature of the particle.

The obtained thermal conductivity enhancement, as well as the prediction from the Maxwell model in Figure 5 shows that the measured thermal conductivity enhancement increases from about 0.630 W/m-k to 0.690 W/m-k with increasing temperature from 100 °C and 500 °C in both nanoparticles and polymer matrix systems, to about 12.5 % volume fraction for the AgNPs. A similar trend but slightly smaller values are predicted by the Maxwell model, which takes into account the effects of the particle volume fraction to obtain thermal conductivity.

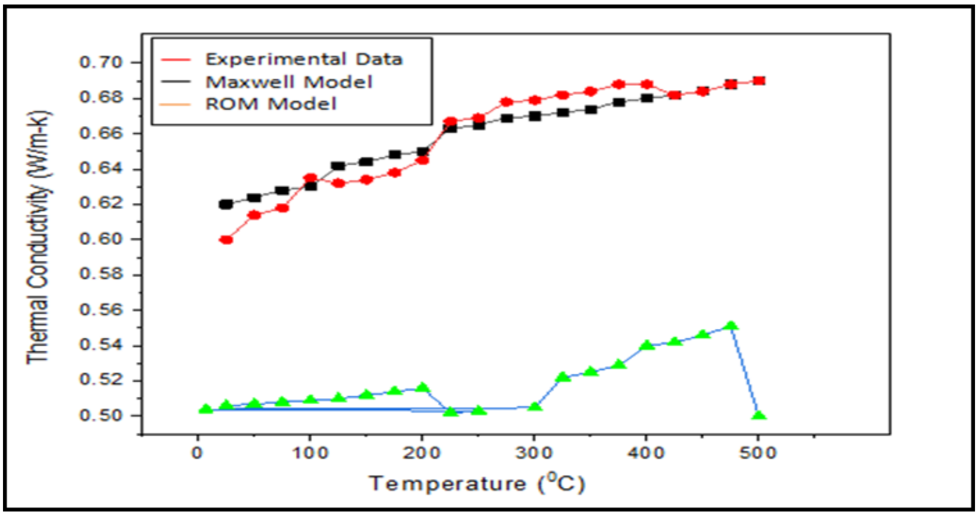

Figure 5. Variation of thermal conductivity of PS/AgNPs with particle temperature obtained for particle volume fraction of 12.5 %

3.2. Contouring of Thermal Conductivity Variations between Particle Volume fraction and Temperature of PS/AgNPs Composite

The Sufer 16 software was used to further show the 2-D contour of thermal conductivity variation over particle volume fraction and temperature of polystyrene silver nanoparticles (PS/AgNPs) composite. Figure 6 show the contour map and the summary of the thermal conductivity variation with the particle volume fraction and temperature of the polystyrene silver nanoparticles PS/AgNPs composite.

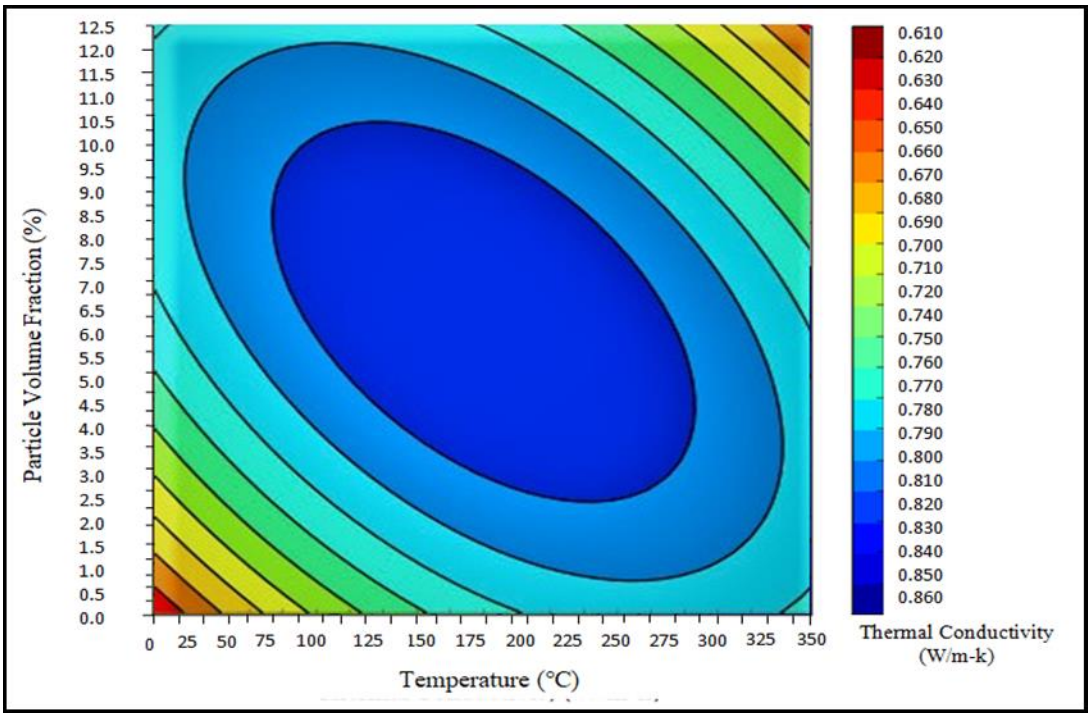

Figure 6. 2-D Contour of Thermal Conductivity Variation over Particle Volume Fraction and Temperature of Polystyrene Silver Nanoparticles (PS/AgNPs) Composite

Figure 6 shows that the temperature between 25 °C to 100 °C has the least value of thermal conductivity with a volume fraction ranging from 0.5 % to 3.0 %. The values of thermal conductivity are between 0.610 W/m-k to 0.680 W/m-k due to low temperature value, as can be seen from the legend, the red and yellow color part of the contour represent the least values of the thermal conductivity of polystyrene silver nanoparticles (PS/AgNPs) composite. Meanwhile towards the temperature between 125 °C to 300 °C have the higher values of the thermal conductivity with volume fraction ranging from 3.5 % to 12.5 %. The values of thermal conductivity are between 0.750 W/m-k to 0. 843 W/m-k as shown from the legend of Figure 8, the green color part and blue color part of the contour represent the higher values of the thermal conductivity which correspond to high temperature values. This result shows that the thermal conductivity of polystyrene silver nanoparticles (PS/AgNPs) composite has indirect and inverse relationship with temperature.

4. Conslussion

In this research work, a mathematical model for calculating the effective thermal conductivity of polystyrene silver nanoparticles PS/AgNPs composite was adopted. A theoretical and analytical Maxwell model for heat conduction has been used, which successfully estimates the effectivethermal conductivity of Polystyrene Silver nanoparticles (PS/AgNPs)composite with filler volume fraction up to 12.5 %. The values obtained from Maxwell model are found to be in good agreement with the experimental results for a set of Polystyrene silver nanoparticles (PS/AgNPs) composites. The Results show that, the thermal conductivity increase with increasing the particle volume fraction concentration. Since our measurements were carried at different increases in temperature, thus, our results show that, interfacial layer between AgNPs, nanoparticles and the volume fraction concentration of particles in the PS base matrix give a significant effect on thermal conductivity of nanoparticles composite. It was suggested that this correlation can be further used for assessment of the effective thermal conductivity of any other similar polymer nanocomposite systems by suitably tuning the value of volume fraction and other parameters into consideration. With light weight and improved thermal conduction capability, this PS/AgNPs nanocomposite can be used for applications such as electronic packages, communication device, thermal grease, thermal interface material and electric cable insulation.

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